

Structural Constraint Integration in Generative Model for Discovery of Quantum Material Candidates

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ABSTRACT

Billions of organic molecules are known, but only a tiny fraction of the functional inorganic materials have been discovered, a particularly relevant problem to the community searching for new quantum materials. Recent advancements in machine-learning-based generative models, particularly diffusion models, show great promise for generating new, stable materials. However, integrating geometric patterns into materials generation remains a challenge. Here, we introduce Structural Constraint Integration in the GENerative model (SCIGEN). Our approach can modify any trained generative diffusion model by strategic masking of the denoised structure with a diffused constrained structure prior to each diffusion step to steer the generation toward constrained outputs. Furthermore, we mathematically prove that SCIGEN effectively performs conditional sampling from the original distribution, which is crucial for generating stable constrained materials. We generate eight million compounds using Archimedean lattices as prototype constraints, with over 10% surviving a multi-staged stability pre-screening. High-throughput density functional theory (DFT) on 26,000 survived compounds shows that over 50% passed structural optimization at the DFT level. Since the properties of quantum materials are closely related to geometric patterns, our results indicate that SCIGEN provides a general framework for generating quantum materials candidates.

Introduction

The structure-property relationships are instrumental in understanding quantum and functional materials, and are a fundamental part of any materials science curriculum. Two key structural indicators, symmetry, and geometric pattern, profoundly influence materials properties. For example, materials with inversion symmetry can lead to topological crystalline insulators¹, whereas breaking inversion symmetry can result in a variety of phenomena such as Rashba spin-orbit coupling², ferroelectricity³, second harmonic generation⁴, and topological Weyl semimetals⁵. Meanwhile, a material's geometric pattern is closely linked to its electronic states and magnetic orderings. The square lattice serves as a prototype for high-temperature cuprate superconductors⁶, while triangular, honeycomb, and kagome lattices can host exotic magnetic states like quantum spin liquids^{7,8}. Additionally, kagome and Lieb lattices can support electronic flat bands^{9,10} with the technological importance of replacing rare-earth elements¹¹. Also, porous structures like zeolite lattices find applications in catalysis¹². However, designing stable materials with desired properties can be nontrivial. For example, only a dozen quantum spin liquid candidates have been identified after a decade of research¹³, and even fewer are known for the Lieb lattice.

Machine-learning (ML) based materials generators have led to a paradigm shift in material design. Diffusion models like CDVAE, UniMat, and DiffCSP^{14–16}, and graph neural network models like GNoME¹⁷, have shown great promise in identifying stable structures to generate millions of materials. However, most ML-based generators create new materials with respect to the distribution of the database, making it challenging to generate materials with specific constraints. Although there have been some developments in the incorporation of crystallographic space groups in the materials generation^{18–20}, the integration of geometric patterns into generation algorithms for functional materials remains challenging. In quantum materials, space group symmetry and geometric patterns can be independent; including the space group symmetry alone will sometimes not allow for proper screening, as is often encountered in monoclinic stacking variants of hexagonal symmetry layers. Moreover, in frustrated magnets, the geometric pattern such as a kagome lattice filled with magnetic atoms plays more important roles than the overall space group in supporting the exotic magnetic structures. Therefore, there is a pressing need to develop an ML-based generator capable of producing new materials constrained by particular geometric patterns.

To answer this need, in this work, we present SCIGEN: Structural Constraint Integration in the GENerative model. SCIGEN is a scheme that can be utilized by any pre-trained generative diffusion model for the incorporation of geometric pattern and symmetry constraints during the generation, without the need for retraining or fine-tuning. Starting from the target constraints, SCIGEN diffuses a random constrained structure over multiple time steps. The constrained structures are used to mask the denoised structure before each diffusion step, creating an inductive bias that directs the generation process toward producing outputs that adhere to the constraints. It turns out that, as we have proven, SCIGEN effectively performs conditional generation with respect to the distribution of the base model. This indicates that the constraint set by SCIGEN would preserve the integrity of the base generative model, including but not limited to the stability of generated materials. To demonstrate, we apply SCIGEN to DiffCSP¹⁶ for generating materials constrained by Archimedean lattices (ALs)^{21,22}, which are a collection of 2D lattice tiling with square, triangular, honeycomb, kagome, and a few other geometric patterns, and rich harbors for exotic quantum materials. We generate a total of 7.87 million materials belonging to ALs. After a four-staged stability pre-screening, over 790,000 materials survived. Structure relaxation on a subset containing 26,000 materials is computed with high-throughput density functional theory (DFT), showing that 95% completed the calculation, and more than 53% can reach the energy minimum within 150 steps of structural optimization. Since SCIGEN requires no extra training apart from the underlying generative model, it also offers a flexible and generically applicable conditioning scheme of materials generation with constraints from both symmetry and geometric patterns.

Results

Structural constraint integration in the generative model

Figure 1 presents the schematic overview of SCIGEN. The goal of crystal structure generation is to find periodic crystals \mathbf{M} , which can be represented by the three components: the lattice matrix containing three basis vectors $\mathbf{L} = [\mathbf{l}_1, \mathbf{l}_2, \mathbf{l}_3] \in \mathbb{R}^{3 \times 3}$, the fractional coordinates $\mathbf{F} = [\mathbf{f}_1, \mathbf{f}_2, \dots, \mathbf{f}_N] \in [0, 1]^{3 \times N}$, and one-hot representations of atom types $\mathbf{A} = [\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_N] \in [0, 1]^{h \times N}$. Our methods impose geometric constraints on \mathbf{L} , \mathbf{F} and \mathbf{A} respectively in diffusion-based material generation. Figure 1a illustrates notable geometries including triangular, honeycomb, and kagome lattices. Following the guideline in Fig. 1b, we initiate the constrained structures with an AL composed of magnetic atoms. Figure 1c explains the algorithm of the generative process integrating the constrained components. The initialized structure is subjected to a diffusion process by adding noise over T -steps denoted as \mathbf{M}_t^c where $t \in [1..T]$ ($T = 1000$ by choice), providing the pre-defined pathway of denoising process for the constrained components. An unconstrained structure is initiated as a completely noisy structure \mathbf{M}_T^u . Both \mathbf{M}_T^c and \mathbf{M}_T^u are integrated to form \mathbf{M}_T . This composite structure \mathbf{M}_T is then denoised to retrieve \mathbf{M}_{T-1}^u . SCIGEN repeats this process through all steps; it merges \mathbf{M}_t^c and \mathbf{M}_t^u to get \mathbf{M}_t , and then predicts \mathbf{M}_{t-1}^u . This iteration optimizes the final material structure \mathbf{M}_0 by guiding a subset of atoms to form AL planar structures. More details are shown in Supplementary Information 3. Additionally, as proven in Supplementary Information 4, SCIGEN can take the structural constraints and fill the remaining unconstrained components, while preserving the integrity of the unconstrained optimization. Following the generation of a large set of material candidates, we evaluate their stability through a four-staged pre-screening process. The pre-screening involves applying chemical rules such as charge neutrality and the volume of atoms occupying the lattice unit cell, along with auxiliary neural networks that predict stability based on the energy above convex hull (E_{hull}) values. After that, we employ high throughput DFT to relax structures and identify potentially stable candidates.

Materials generation with Archimedean lattice constraints

Figures 2a-c display the results of materials generation constrained by three primary AL types: (a) triangular, (b) honeycomb, and (c) kagome. The AL structures are formed in the generated structures, as SCIGEN algorithm has guided them to be formed as pre-defined. The positions of the other unconstrained atoms are not specified rigorously but are often found to reside on the sites that bridge the AL atoms. For triangular lattices (Fig. 2a), each of the unconstrained atoms is placed on the sites connecting with three magnetic atoms forming an equilateral triangle. For honeycomb lattices (Fig. 2b), we often observe

materials with one unconstrained atom at the center of the hexagon formed with magnetic atoms within the same plane. As to kagome materials (Fig. 2c), unconstrained atoms bridge the equilateral triangles and the hexagons of kagome lattice layers. If the space inside the polygons is too small compared to the atomic radii, the filler atoms will be pushed outside the AL plane. On the other hand, large polygons like hexagons can accommodate the filler atoms to fit within the same plane.

To generate constrained material structures with a higher likelihood of stability, we develop a scheme for sampling initial conditions. We analyze the ratio of stable outputs, defined as the survival ratio after the multi-staged pre-screening processes. First, we sample the number of atoms per unit cell (N) from a uniform distribution to identify which N values are more likely to pass the stability pre-screening. This results in a probability distribution p_N values based on their pre-screened stability. We then use this probability distribution p_N to sample N for initializing the large-scale generative process. Figure 2d shows the sampling profile of N , which covers all of the 10 common magnetic atoms as the vertices of AL structures. For triangular lattice materials, smaller N values show higher success rates, whereas larger N values are favored for honeycomb and kagome. This result is reasonable since the AL type is directly linked to the unit cell size, which is a linear function of bond lengths for each class of AL types. For triangular lattice, the lattice parameters l_1 and l_2 are the same as the bond length of the neighbor node, while for honeycomb and kagome lattices, the lattice parameters are $\sqrt{3}$ and 2 times of the bond length, respectively. In the case where many atoms are packed into the unit cell of a small cross-section of the AL, the cell needs to be “tall”, i.e., l_3 needs to be larger with respect to l_1 and l_2 . Next, we survey which magnetic atoms are suitable as the vertices of ALs. Figure 2e presents the number of stable materials after the prescreening with respect to magnetic atom types, which we analyze from the set of 3000 generated materials for each lattice type and each magnetic atom. Despite variations, all magnetic atoms are shown to be able to form AL structures. Therefore, we choose to sample atom types for AL vertices with equal probabilities for large-scale materials generation and database construction. Methods section and Supplementary Information 2 describe in detail the sampling schemes for the initialization conditions.

Our exploration of materials with geometrical constraints does not end with the three primary types of ALs but can apply to other geometrical patterns. In contrast to the common types of triangular, honeycomb, and kagome lattices, magnetic systems known to fit in other ALs are extremely rare. Figure 3 showcases $3 \times 3 \times 1$ supercells of the generated materials with seven other types of Archimedean lattices: Square, Elongated triangular, Snub square, Truncated square, Small rhombitrihexagonal, Snub hexagonal, and Truncated hexagonal. One type of AL lattice, Great rhombitrihexagonal, is not presented due to the challenge to generate stable materials. The unconstrained atoms within these materials often play a critical role in the overall stability of the structures. They tend to bridge gaps between structured lattice layers, either by sitting at the center of polygons on the same plane or contacting all vertices of the polygon structures, effectively stabilizing the AL layers. This bridging is not just a passive consequence of the material generation process but actively contributes to the mechanical and thermal stability of materials²³. Interestingly, even when not explicitly constrained to form specific lattice structures, these unconstrained atoms frequently organize into recognizable Archimedean patterns. This trend could suggest an inherent preference or stability in the configurations of AL whose vertices are equivalent with respect to the local coordinates.

Materials generation with Lieb-like lattice structures

The Lieb lattice is a variation of AL that consists of a square lattice with additional atoms located at the centers of each edge of the squares, as visualized in Fig. 4a. Each unit cell of the Lieb lattice contains three atoms. The geometry of the Lieb lattice can lead to magnetic frustration when interacting spins are placed at each lattice site, as we expect for AL structures. This can result in complex magnetic states, which are of significant interest for studying quantum magnetism. Beyond that, Lieb lattices are studied to possess characteristic electronic properties. One key feature of the Lieb lattice is the presence of a flat electronic band¹⁰. Contrary to localized atomic orbitals, the flat bands formed from the Lieb lattice originate from the destructive quantum interference effect which quenches the kinetic energy. This may lead to interesting physical phenomena such as enhanced electron correlation and high-temperature superconductivity^{24,25}. Also, recent research has shown that the Lieb lattice can exhibit non-trivial topological properties when subjected to various perturbations²⁶. However, the Lieb lattice has mainly been achieved in artificial systems like photonic crystals^{27,28}, and atomic solids that can host Lieb lattice are extremely rare.

In this work, we also focus on the Lieb-like lattice where magnetic atoms sit on the Lieb lattice. Figures 4b,c show the generated materials with Lieb-lattice-based crystal structures and their calculated band structures. In these generated materials, magnetic atoms such as terbium (Tb) and dysprosium (Dy) are strategically positioned at the nodes of the Lieb lattice. Following structural relaxation through DFT calculations, the integrity of the Lieb lattice architecture is maintained, and the structures exhibit the anticipated flat-band characteristics close to the Fermi level. These outcomes demonstrate SCIGEN’s ability to generate new, stable materials with exotic geometric patterns, even when there are very few known materials that fit the desired geometric pattern.

Database of the materials with Archimedean lattice

As detailed in Supplementary Information 7, we generate an AL materials database using SCIGEN. The database contains three components: the total 7.87 million materials generated by the SCIGEN model, the 790 thousand materials that survived four

stages of stability pre-screening processes, and 24,743 out of 26,000 sub-sampled materials in which DFT calculations are successfully converged. By systematically extending our exploration to encompass a wider range of ALs, we can investigate new exotic magnetic orderings, discover porous structures beyond zeolites, and explore new electronic flatband structures, among other possibilities.

Conclusions

In this work, we present SCIGEN, a new generative model aimed at discovering quantum material candidates that adhere to geometric constraints. Our method leverages an AL layer within the crystal structure to identify potential quantum materials. These materials have been validated through DFT to ensure that their relaxed structures are consistent with the machine-learning generations.

To further enhance the validity of SCIGEN, it is crucial to conduct experimental verification through the synthesis of these machine-generated materials. Computation-aided synthesizability check may involve additional analysis in binary, ternary, or other more complex phase diagrams. Setting aside experimental validation, SCIGEN paves an avenue for a few future directions. By focusing on atomic arrangements, we can explore additional geometry-related constraints, such as bonding types, coordination numbers, short-range orderings, and point-group and space group symmetries, during materials generation. Additionally, integrating other diffusion channels, like through the virtual node approach, allows us to incorporate more complex constraints such as defect constraints and magnetic interaction constraints, broadening the scope of the SCIGEN model. Moreover, conditioning the generation process with targeted functionalities, such as specific electrical and optoelectronic properties, or sustainability or environmental impact of materials, can lead to the direct creation of materials with tailored performance. Our SCIGEN model represents a general machine learning-based framework for discovering new quantum materials. It leverages information typically absent from crystal structure databases, offering deeper insights into the structure-property relationships of emerging quantum materials.

Methods

Initialization of the Archimedean Lattices

We describe the workflow to initialize the materials generation process related to the both AL and the entire structure of crystal for the diffusion model. This initialization process involves a few steps: the choice of AL, the atom types, and the total number of atoms per unit cell. Here we provide a summary of the initialization process in Fig. 2b, where more detailed scheme can be found in Supplementary Information 2.

First, we assign the required geometric domain condition to the crystals. In SCIGEN, we specify one of the AL structures, such as triangular, honeycomb, or kagome lattice, as geometric domain condition. Each type of AL requires the number of vertices per unit cell and the size of the unit cell. Supplementary Information 1 presents the geometric patterns and the preliminary profiles of all AL and Lieb lattices.

Second, we choose the constrained atom type \mathcal{A}^c placed on the vertices of the AL structure assigned above. To generate candidate materials which may host geometrically frustrated quantum magnetism, we specify 10 types of common magnetic atoms (Mn, Fe, Co, Ni, Ru, Nd, Gd, Tb, Dy, Yb) on the vertices. The atom types are chosen independently from the AL choice above.

Third, we sample the constrained magnetic bond lengths d^c , aka the distances between the nearest-neighbor magnetic atoms forming the ALs. For each magnetic atom type \mathcal{A}^c , we generated the profile of the bond lengths by sampling the nearest-neighbor distances between the corresponding atoms in the MP-20 dataset^{29,30} using CrystalNN³¹. To ensure the nearest-neighbor distances do not become significantly close, we cut the minimum lengths by the metallic radii³² for each atom type. The bond length distribution for each magnetic atom type \mathcal{A}^c , $p_{dc}(\mathcal{A}^c)$, is presented in Supplementary Information 2.

Finally, we sample the total number of atoms per unit cell N . Each of the ALs has the distribution of the preferable N values with better stability. We generate p_N , the stable materials probability distribution of N . We can sample N from p_N as the sampling profile of N for each AL type. The sampling profile of both p_N and $p_N(\mathcal{A}^c)$, which is distribution of with each magnetic atom type \mathcal{A}^c , are displayed in Supplementary Information 2.

To impose Archimedean lattice as the constraints, we organize masks $\mathbf{m} = (\mathbf{m}^L, \mathbf{m}^F, \mathbf{m}^A)$, which give constraints to the lattice L , fractional coordinates F , and atom types A respectively. \mathbf{m}^L is equal to 1 for the two lattice basis vectors \mathbf{l}_1 and \mathbf{l}_2 , defining the unit cell of AL layer plane. \mathbf{m}^L is equal to 0 for \mathbf{l}_3 , as we let the diffusion model generate \mathbf{l}_3 without explicit constraints. We assign \mathbf{m}^F is equal to 1 for the i -th atoms ($i \in [1, N^c]$) to guide them to be placed at the vertex positions of AL layers. The same rule applies for \mathbf{m}^A so that the atoms at AL vertices result in the magnetic atom types \mathcal{A}^c .

Integration of constrained and unconstrained components to guide materials generation

We design SCIGEN as a generic framework applicable for any diffusion model as a base model. Without loss of generality, let the pre-trained base model represent a periodic structure as \mathbf{M}_0 , with T diffusion steps, a sampling probability prior P_T , diffusion inference model q , which is normally chosen to map the materials distribution of the training dataset to P_T , and denoising generative model p which needs to be trained. The diffusion inference model q works by iteratively injecting noise to the input structure, \mathbf{M}_0 . The inference probability of most diffusion models is a Markov process, i.e., the probability of diffusing \mathbf{M}_0 for t steps to \mathbf{M}_t can be written as

$$P(\mathbf{M}_t | \mathbf{M}_0) = q_{0,t}(\mathbf{M}_t | \mathbf{M}_0) = \prod_{s=1}^t q_{s-1,s}(\mathbf{M}_s | \mathbf{M}_{s-1}) \quad (1)$$

with

$$P(\mathbf{M}_T | \mathbf{M}_0) = q_{0,T}(\mathbf{M}_T | \mathbf{M}_0) \approx P_T. \quad (2)$$

A well-trained diffusion model should have denoising generative model p that can inverse the diffusion, i.e., for a denoising step from \mathbf{M}_t to \mathbf{M}_{t-1} ,

$$p_{t,t-1}(\mathbf{M}_{t-1} | \mathbf{M}_t) \approx q_{t,t-1}(\mathbf{M}_{t-1} | \mathbf{M}_t). \quad (3)$$

Here, the subscripts of p and q indicate the initial and final time steps that the models are applied to, e.g., q_{t_1,t_2} is the diffusion inference from time step t_1 to t_2 . Note that, since q is normally chosen to be a simple probabilistic function, we cannot easily find its inverse. Hence, the training for the denoising generative model is required.

Our approach to material design is summarized in Algorithm 1, where integration of geometrical constraints plays a pivotal role in ensuring that certain structural elements, like lattice configurations or specific atomic distributions, adhere closely to predefined parameters. This method effectively blends prescribed structural characteristics with the creative latitude allowed in other aspects of the material's architecture. Previously, a generative model with unmasked areas as constraints has been employed in image generation for image inpainting, such as RePaint method³³. However, the geometrical pattern constraint for crystal generation is still challenging and differs in a few ways. The generation of crystal generative model with geometrical constraint involves several key steps:

1. **Adding noise to the constraint structures:** Initially, we introduce noise to a structure which is randomly selected from structures that satisfy the target constraints (This constrained structure can be unstable, or unrealistic as long as it contains the target constraints.) with the diffusion inference model, q , to get diffused constrained structures for each time step $t \in [1, T]$. This operation is aimed at creating a predefined pathway for denoising the constrained structures. The unconstrained components of the crystals are guided by this known denoising pathway, which results in the presence of constrained components in the final outputs.
2. **Denoising the unconstrained structures with a base diffusion model:** Concurrently, the parts of the structure that are unconstrained from these specific constraints undergo a normal denoising process with p . This process, facilitated by the base model, iteratively refines these regions by methodically reducing the introduced noise, thereby nudging them toward physically realistic configurations.
3. **Integration of the constrained and unconstrained structures:** For each denoising step, after processing both parts independently, they are carefully recombined. This combination is critical as it ensures the integrity of the predefined constraints is maintained while integrating seamlessly with the freely generated segments. This method preserves essential structural features and fosters innovation in material design.

Algorithm 1 presents the SCIGEN sampling procedure designed to generate material structures with structural constraints. The algorithm utilizes a diffusion model to iteratively refine structures, ensuring the generated structures contain specific geometry as constraints. The procedure begins with the initialization of constrained structures, indicated with superscript c , \mathbf{M}_0^c , along with the corresponding masks \mathbf{m} , which indicate the constrained components in \mathbf{M}_0^c with binary masking, i.e., assigns value of 1 to constrained, and 0 to the unconstrained components. The final-time-step unconstrained structure, indicated with superscript u , \mathbf{M}_T^u , and constrained structure \mathbf{M}_T^c are sampled from the probability prior P_T of the base model. Through masking, we obtain the final-time-step structure \mathbf{M}_T that contains the constrained components from \mathbf{M}_T^c , and the remaining parts from \mathbf{M}_T^u formulated as $\mathbf{M}_T \leftarrow \mathbf{m} \odot \mathbf{M}_T^c + (1 - \mathbf{m}) \odot \mathbf{M}_T^u$ where \odot represents a component-wise multiplication. Basically, the components of \mathbf{M}_T that got masked (values in \mathbf{m} equal to 1) come from \mathbf{M}_T^c while the remaining components (values in \mathbf{m} equal to 0) come from \mathbf{M}_T^u .

The iterative process begins from the final time step T and proceeds backward to 0. For each time step t , the structure \mathbf{M}_t undergoes the denoising process giving the distribution of the unconstrained structure at time step $t - 1$, \mathbf{M}_{t-1}^u , as $p_{t,t-1}(\mathbf{M}_{t-1}^u | \mathbf{M}_t)$. Concurrently, the diffusion process gives the distribution of the constrained structure \mathbf{M}_{t-1}^c as $q_{0,t-1}(\mathbf{M}_{t-1}^c | \mathbf{M}_0)$. Then, the unconstrained structure \mathbf{M}_{t-1}^u , and constrained structure \mathbf{M}_{t-1}^c are sampled from their corresponding probability distributions. The structure \mathbf{M}_t is updated by combining the sampled constrained and unconstrained parts using the mask \mathbf{m} similar to the final-time-step case. The process continues iteratively until the initial time step is reached, at which point the refined structure \mathbf{M}_0 is returned. This ensures that the generated material structures respect the given constraints and exhibit realistic and viable configurations. Supplementary Information 3 provides the schematic explanation of the denoising process, as well as the integration of constrained and unconstrained components of material structures.

This approach effectively integrates structural constraints into the diffusion model, enabling the generation of novel material structures that align with the AL structures as the predefined requirements. Using masks to combine constrained and unconstrained parts ensures that the constraints are maintained throughout the iterative refinement process, resulting in high-quality material structures suitable for practical applications.

Algorithm 1 Structural Constraint Integration in Material Generation Procedure

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1: Input: constrained structure  $\mathbf{M}_0^c$ , constraint mask  $\mathbf{m}$ , diffusion inference model  $q$ , denoising generative model  $p$ , number of steps  $T$ , probability prior  $P_T$ 
2: Sample  $\mathbf{M}_T^u \sim P_T$ ,  $\mathbf{M}_T^c \sim P_T$ 
3:  $\mathbf{M}_T \leftarrow \mathbf{m} \odot \mathbf{M}_T^c + (1 - \mathbf{m}) \odot \mathbf{M}_T^u$ 
4: for  $t = T, \dots, 1$  do
5:   Sample  $\mathbf{M}_{t-1}^c \sim q_{0,t-1}(\mathbf{M}_{t-1}^c | \mathbf{M}_0)$ 
6:   Sample  $\mathbf{M}_{t-1}^u \sim p_{t,t-1}(\mathbf{M}_{t-1}^u | \mathbf{M}_t)$ 
7:    $\mathbf{M}_{t-1} \leftarrow \mathbf{m} \odot \mathbf{M}_{t-1}^c + (1 - \mathbf{m}) \odot \mathbf{M}_{t-1}^u$ 
8: return  $\mathbf{M}_0$ .

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To demonstrate the algorithm for the generation of AL materials, we chose DiffCSP¹⁶ as the base model of SCIGEN before applying geometric constraint. In DiffCSP, the structure representation got divided into three components $\mathbf{M} = (\mathbf{L}, \mathbf{F}, \mathbf{A})$: the lattice matrix containing three basis vectors $\mathbf{L} = [\mathbf{l}_1, \mathbf{l}_2, \mathbf{l}_3] \in \mathbb{R}^{3 \times 3}$, the fractional coordinates $\mathbf{F} = [\mathbf{f}_1, \mathbf{f}_2, \dots, \mathbf{f}_N] \in [0, 1)^{3 \times N}$, and one-hot representations of atom types $\mathbf{A} = [\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_N] \in [0, 1]^{h \times N}$. Using these components, the infinite periodic crystal can be described as

$$\{(\mathbf{a}_i, \mathbf{x}_i) \mid \mathbf{x}_i = \mathbf{L} \cdot (\mathbf{f}_i + \mathbf{k}), \forall \mathbf{k} \in \mathbb{Z}^{3 \times 1}, \forall i \in [1..N]\} \quad (4)$$

which tell all atomic types \mathbf{a} , and Cartesian coordinates \mathbf{x} of every atoms in the structure. DiffCSP uses normalized Gaussian diffusion in its diffusion inference model q which have standard normal distribution as probability prior, i.e., $P_T = \mathcal{N}(0, I)$. Furthermore, the diffusion is applied independently between components, making it possible to split the model as $q = (q^{\mathbf{L}}, q^{\mathbf{F}}, q^{\mathbf{A}})$ where the superscripts indicate the components that the diffusion acts on. We can write the split diffusion inference model of DiffCSP as

$$q_{t,t+1}(\mathbf{M}_{t+1} | \mathbf{M}_t) = q_{t,t+1}^{\mathbf{L}}(\mathbf{L}_{t+1} | \mathbf{L}_t) \cdot q_{t,t+1}^{\mathbf{F}}(\mathbf{F}_{t+1} | \mathbf{F}_t) \cdot q_{t,t+1}^{\mathbf{A}}(\mathbf{A}_{t+1} | \mathbf{A}_t). \quad (5)$$

Since the denoising generative process of DiffCSP utilizes Predictor-Corrector sampling³⁴ mechanism on the fractional coordinate components only, the model need to be split into $p = (p^{\mathbf{L}}, p^{\mathbf{F},p}, p^{\mathbf{F},c}, p^{\mathbf{A}})$ where the boldface superscripts indicates the components that the diffusion gives while p and c superscripts indicate predictor and corrector sub-models, respectively. We can write the split denoising generative model of DiffCSP as

$$p_{t,t-1}(\mathbf{M}_{t-1} | \mathbf{M}_t) = p_{t,t-1}^{\mathbf{L}}(\mathbf{L}_{t-1} | \mathbf{M}_t) \cdot p_{t,t-1}^{\mathbf{F},p}(\mathbf{F}_{t-\frac{1}{2}} | \mathbf{M}_t) \cdot p_{t,t-1}^{\mathbf{F},c}(\mathbf{F}_{t-1} | \mathbf{L}_{t-1}, \mathbf{F}_{t-\frac{1}{2}}, \mathbf{A}_{t-1}) \cdot p_{t,t-1}^{\mathbf{A}}(\mathbf{A}_{t-1} | \mathbf{M}_t). \quad (6)$$

Basically, the lattice, and atomic type components got denoised by their respective model to get \mathbf{L}_{t-1} , and \mathbf{A}_{t-1} , respectively. For the fractional coordinate components, the predictor denoises them to the half-time-step point $\mathbf{F}_{t-\frac{1}{2}}$, and the corrector uses $\mathbf{F}_{t-\frac{1}{2}}$, \mathbf{L}_{t-1} , and \mathbf{A}_{t-1} to predict \mathbf{F}_{t-1} . Because of this additional prediction of $\mathbf{F}_{t-\frac{1}{2}}$, algorithm 1 need to be slightly modified to accommodate the constraints that are also imposed on the $\mathbf{F}_{t-\frac{1}{2}}$ as shown in algorithm 2.

Pre-screening procedure to retrieve stable materials structures

Following the generation of materials constrained by AL structures, it becomes essential to evaluate their stability. Due to the high volume of generated candidates—often reaching into the millions—a rapid yet reliable method is necessary to assess stability. Here, we describe our four-staged pre-screening of materials based on a series of stability criteria.

Algorithm 2 Structural Constraint Integration in Material Generation with DiffCSP

- 1: **Input:** constrained structure $\mathbf{M}_0^c = (\mathbf{L}_0^c, \mathbf{F}_0^c, \mathbf{A}_0^c)$, constraint mask $\mathbf{m} = (\mathbf{m}^L, \mathbf{m}^F, \mathbf{m}^A)$, diffusion inference model $q = (q^L, q^F, q^A)$, denoising generative model $p = (p^L, p^{F,p}, p^{F,c}, p^A)$, number of steps T
- 2: Sample $\mathbf{M}_T^u = (\mathbf{L}_T^u, \mathbf{F}_T^u, \mathbf{A}_T^u) \sim \mathcal{N}(0, I)$, $\mathbf{M}_T^c = (\mathbf{L}_T^c, \mathbf{F}_T^c, \mathbf{A}_T^c) \sim \mathcal{N}(0, I)$
- 3: $\mathbf{M}_T = (\mathbf{L}_T, \mathbf{F}_T, \mathbf{A}_T) \leftarrow \mathbf{m} \odot \mathbf{M}_T^c + (1 - \mathbf{m}) \odot \mathbf{M}_T^u$
- 4: **for** $t = T, \dots, 1$ **do**
- 5: Sample $\mathbf{M}_{t-1}^c = (\mathbf{L}_{t-1}^c, \mathbf{F}_{t-1}^c, \mathbf{A}_{t-1}^c) \sim q_{0,t-1}(\mathbf{M}_{t-1}^c | \mathbf{M}_0^c)$
- 6: Sample $\mathbf{L}_{t-1}^u \sim p_{t,t-1}^L(\mathbf{L}_{t-1}^u | \mathbf{M}_t)$, $\mathbf{A}_{t-1}^u \sim p_{t,t-1}^A(\mathbf{A}_{t-1}^u | \mathbf{M}_t)$
- 7: $\mathbf{L}_{t-1} \leftarrow \mathbf{m}^L \odot \mathbf{L}_{t-1}^c + (1 - \mathbf{m}^L) \odot \mathbf{L}_{t-1}^u$
- 8: $\mathbf{A}_{t-1} \leftarrow \mathbf{m}^A \odot \mathbf{A}_{t-1}^c + (1 - \mathbf{m}^A) \odot \mathbf{A}_{t-1}^u$
- 9: Sample $\mathbf{F}_{t-\frac{1}{2}}^c \sim q_{0,t-1}^F(\mathbf{F}_{t-1}^c | \mathbf{F}_0^c)$
- 10: Sample $\mathbf{F}_{t-\frac{1}{2}}^u \sim p_{t,t-1}^{F,p}(\mathbf{F}_{t-\frac{1}{2}}^u | \mathbf{M}_t)$
- 11: $\mathbf{F}_{t-\frac{1}{2}} \leftarrow \mathbf{m}^F \odot \mathbf{F}_{t-\frac{1}{2}}^c + (1 - \mathbf{m}^F) \odot \mathbf{F}_{t-\frac{1}{2}}^u$
- 12: Sample $\mathbf{F}_{t-1}^u \sim p_{t,t-1}^{F,c}(\mathbf{F}_{t-1}^u | \mathbf{L}_{t-1}, \mathbf{F}_{t-\frac{1}{2}}, \mathbf{A}_{t-1})$
- 13: $\mathbf{F}_{t-1} \leftarrow \mathbf{m}^F \odot \mathbf{F}_{t-1}^c + (1 - \mathbf{m}^F) \odot \mathbf{F}_{t-1}^u$
- 14: **return** $\mathbf{M}_0 = (\mathbf{L}_0, \mathbf{F}_0, \mathbf{A}_0)$.

Charge Neutrality

Materials must be electrically neutral to ensure stability and real-world applicability. We employed the SMACT approach³⁵ to evaluate the charge neutrality of generated materials. This process, inspired by methodologies described in the CDVAE approach¹⁴, ensures that only chemically feasible materials are considered in subsequent steps.

Density and Space Occupancy Ratio

Some generated materials feature densely packed atomic configurations, which are unrealistic in actual crystalline phases. To address this, we compare these materials against a reference dataset (MP-20) to identify and eliminate those with excessively high atom densities. The space occupancy ratio R_{occ} is calculated as

$$R_{occ} = \frac{\sum_{i=1}^N \frac{4\pi r_i^3}{3}}{V_{cell}} \quad (7)$$

where r_i is the radius of the i -th atom and V_{cell} is the volume of the unit cell. Materials in MP-20 observed a similar distribution of R_{occ} that is independent of N , as we can find in Supplementary Information 6. We discard materials with an R_{occ} value exceeding 1.7, a threshold based on the distribution of R_{occ} in the MP-20 dataset.

Graph Neural Network Classifiers for Stability Evaluation

To rapidly assess the stability of the remaining material candidates, we utilize graph neural networks (GNNs) based on the E3NN^{36,37} framework, designed for their efficiency in handling crystallographic data. We develop two models:

- **GNN for Stability classification Ψ_1 :** This model predicts whether a material's energy above the convex hull (E_{hull}) is below a threshold of 0.1 eV, which is indicative of thermodynamic stability. The model is trained using data from the Matbench-discovery³⁸.
- **GNN for Stability classification Ψ_2 :** Recognizing the potential for our model to generate materials that diverge from known stable structures, this classifier distinguishes between pristine and diffused structures. Training data includes original structures from the MP-20 dataset and the ones with added Gaussian noise on unit cell matrix \mathbf{L} and fractional coordinates \mathbf{F} , simulating potential inaccuracies in atomic positions during generation. As the training dataset of Ψ_2 , we diffuse \mathbf{L} and \mathbf{F} as $\mathbf{L}' = \mathbf{L} + (l_1, l_2, l_3)^T \cdot \mathcal{N}(0, \sigma_d^2 I)$ and $\mathbf{F}' = w(\mathbf{F} + \mathcal{N}(0, \sigma_d^2 I))$, respectively. Here, σ_d regulates the level of diffusion, and $w(\cdot)$ is a wrapping function that adjust fractional coordinates to fit within [0, 1]. We decide that 1% diffusion materials ($\sigma_d = 0.01$) are stable, but 5% diffusion materials ($\sigma_d = 0.05$) are unstable. This model helps ensure that even stable materials are not overly distorted or unrealistic.

The two GNN-based classifiers are in simple architecture, but presented high accuracy. We present the confusion matrices of the two models in Supplementary Information 6. The prediction accuracy for the test dataset is 0.83 and 0.99, respectively.

The four-staged pre-screening filters could provide us with an extremely efficient screening tool to evaluate the stability of the generated materials. We argue this stability evaluation is valid, as we observe the materials gain stability as it goes through the denoising process from the noisy structures (\mathbf{M}_T) to the pristine ones (\mathbf{M}_0). Moreover, more than 50% of pre-screened materials survive DFT relaxation, indicating the efficacy of the pre-screening process. The detail of the stability evaluation is shown in Supplementary Information 6.

DFT for stability evaluation and structural relaxation

The candidate models are further evaluated with DFT for potential structural stability. Due to the high cost of DFT calculations, it is necessary to balance the accuracy and throughput. In the first stage of DFT screening, we choose to use a relatively coarse treatment of the electronic structure to evaluate as many candidates as possible (up to 26,000). Planewave DFT calculations are performed using the Vienna Ab initio Simulation Package (VASP)³⁹. The calculation used Projector Augmented Wave (PAW) method^{40,41} to describe the effects of core electrons and Perdew-Burke-Ernzerhof (PBE)⁴² implementation of the Generalized Gradient Approximation (GGA) for the exchange-correlation functional. The energy cutoff is $1.2 \cdot \text{max(ENMAX)}$ for the plane-wave basis of the valence electrons. The electronic structure is calculated on Γ -centered mesh for the unit cell (the grid length density is $5 k\text{-points per nm}^{-1}$). The total energy tolerance for electronic energy minimization is 10^{-6} eV, and the energy criterion for structure optimization is 10^{-5} eV. The maximum number of steps is 60 for electronic self-consistent calculation and 150 for structural optimization. During the structural relaxation, the symmetry of the crystal is maintained while the cell shape/size and all atomic coordinates are allowed to relax. Non-spin-polarized calculation is employed for this initial screening. A small fraction of models failed the electronic structure calculation, which are terminated and the corresponding candidates are considered unstable. For the candidates with completed VASP calculation (either because the energy criterion is reached or the maximum number of relaxation steps is reached), the following quantities are extracted/calculated as indicators of potential stability: (1) maximum interatomic force after relaxation, (2) initial and final total energy, (3) average changes in lattice constants, (4) average changes in atomic coordinates. These quantities are then analyzed and compared to identify potentially stable candidates worth further and more rigorous evaluations.

Band structure calculation for Lieb-like lattice materials

The DFT band structure calculations for Lieb-like lattice structures are performed using VASP. PAW method and PBE exchange-correlation functional are used for all DFT calculations. The initial electronic structure calculations are performed on a K-point mesh centered at Gamma point with resolved value $k_{mesh} = 0.03 \cdot 2\pi/\text{\AA}$ for each structure. The band structure is subsequently calculated on a high symmetry path generated by the VASPKIT code⁴³.

Data visualization

We use VESTA⁴⁴ to visualize the materials structures presented in the main article. For Supplementary Information, we utilize OVITO⁴⁵ to visualize the materials structures.

Data Availability Statement

We compile a comprehensive database of AL materials generated by SCIGEN. The dataset provides the folders of the entire generated materials (7.87 million), the survived materials after the four-staged pre-screening process (790 thousand materials), and DFT-relaxed structures (24,743). The folder with DFT calculation contains materials structures before and after relaxation. The Supplementary dataset is available in Figshare repository⁴⁶.

Code Availability Statement

The source code is available at (<https://github.com/RyotaroOKabe/SCIGEN>).

Acknowledgements

RO and ML thank C Batista, A Christianson, F Frenkel, A May, R Moore, B Ortiz, and F Ronning for the helpful discussion. RO acknowledges the support from the U.S. Department of Energy (DOE), Office of Science (SC), Basic Energy Sciences (BES), Award No. DE-SC0021940 and Heiwa Nakajima Foundation. AC acknowledges support from National Science Foundation (NSF) Designing Materials to Revolutionize and Engineer our Future (DMREF) Program with Award No. DMR-2118448. BH and YC are partially supported by the Artificial Intelligence Initiative as part of the Laboratory Directed Research and Development (LDRD) program of Oak Ridge National Laboratory (ORNL), managed by UT-Battelle, LLC, for the US Department of Energy under Contract DE-AC05-00OR22725. Computing resources for a portion of the work were made available through the VirtuES project, funded by the LDRD Program and Compute and Data Environment for Science (CADES) at ORNL. Another portion of simulation results were obtained using the Frontera computing system at the Texas Advanced

Computing Center. ML acknowledges the support from NSF ITE-2345084, the Class of 1947 Career Development Chair, and the support from R. Wachnik.

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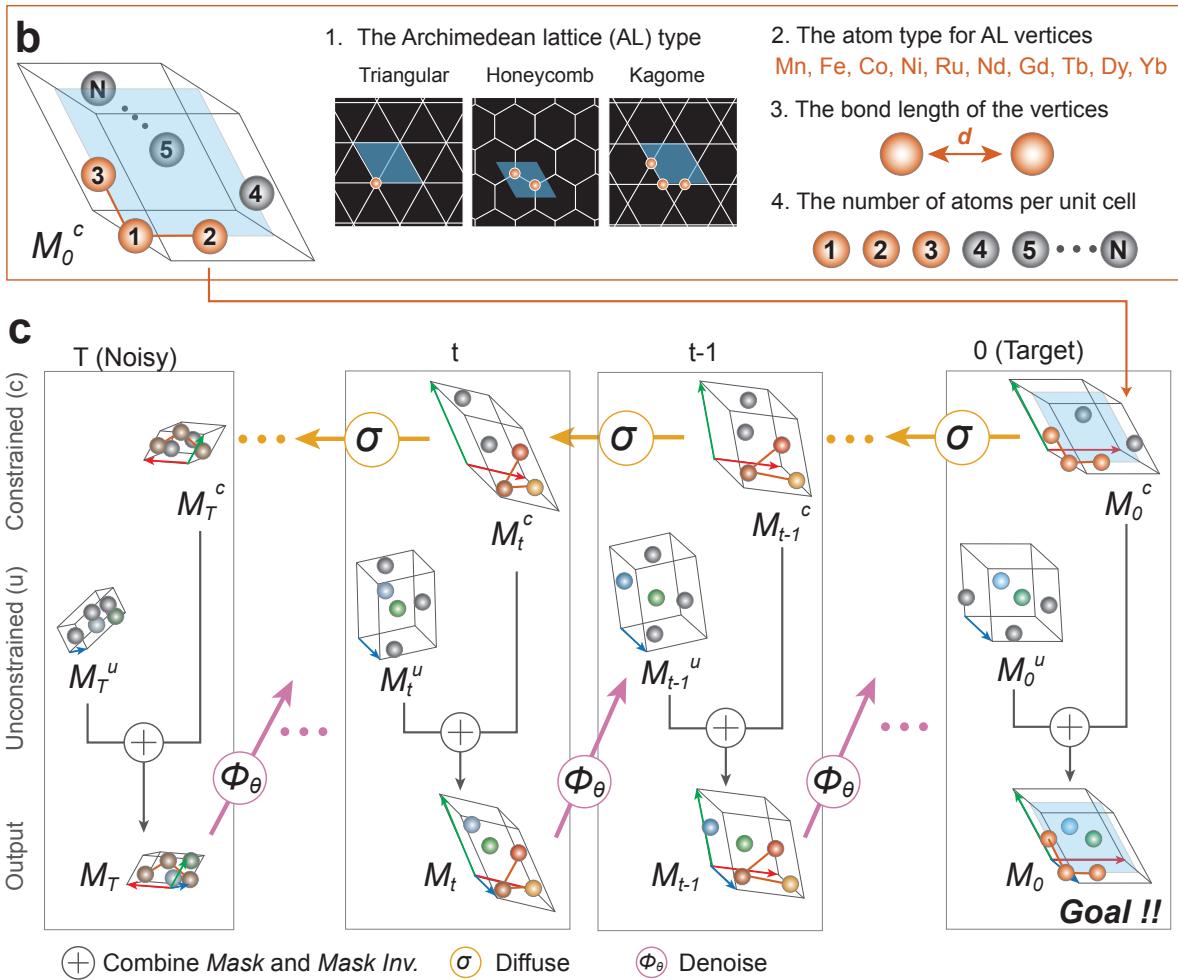
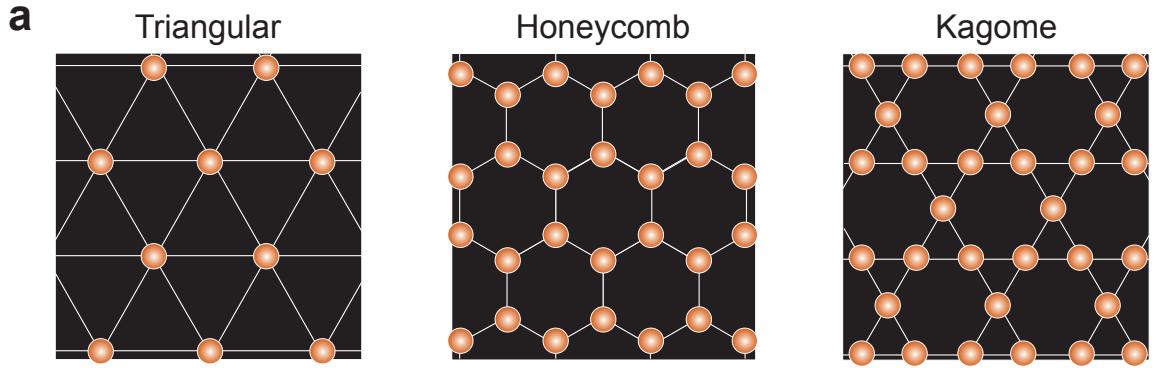


Figure 1. Schematic overview of material generation with geometric patterns as constraints. **a.** Three primary classes of Archimedean lattices with hexagonal unit cells: triangular, honeycomb, and kagome. **b.** Guideline for structure initialization for diffusion model, with magnetic atoms at Archimedean lattice vertices. Required components include: (1) lattice types, (2) magnetic atom types, (3) nearest-neighbor distances, and (4) total number of atoms per unit cell. **c.** Methodology of crystal structure generation via diffusion denoising probabilistic model with geometrical pattern as constraints. The initialized structures are iteratively made noisy (σ), to prepare predefined pathway of the constrained structure \mathbf{M}_t^c , $t \in [1, T]$. For each denoising step t , an unconstrained structure \mathbf{M}_t^u is combined with constrained structure \mathbf{M}_t^c to get an integrated structure \mathbf{M}_t . \mathbf{M}_t is passed to the denoising model Φ_θ and denoised to become the unconstrained structure \mathbf{M}_{t-1}^u . By repeating this process, we obtain the final crystal structure \mathbf{M}_0 , which is guided by the geometrical pattern constraints \mathbf{M}_0^c but remains realistic with a fair chance to maintain stability.

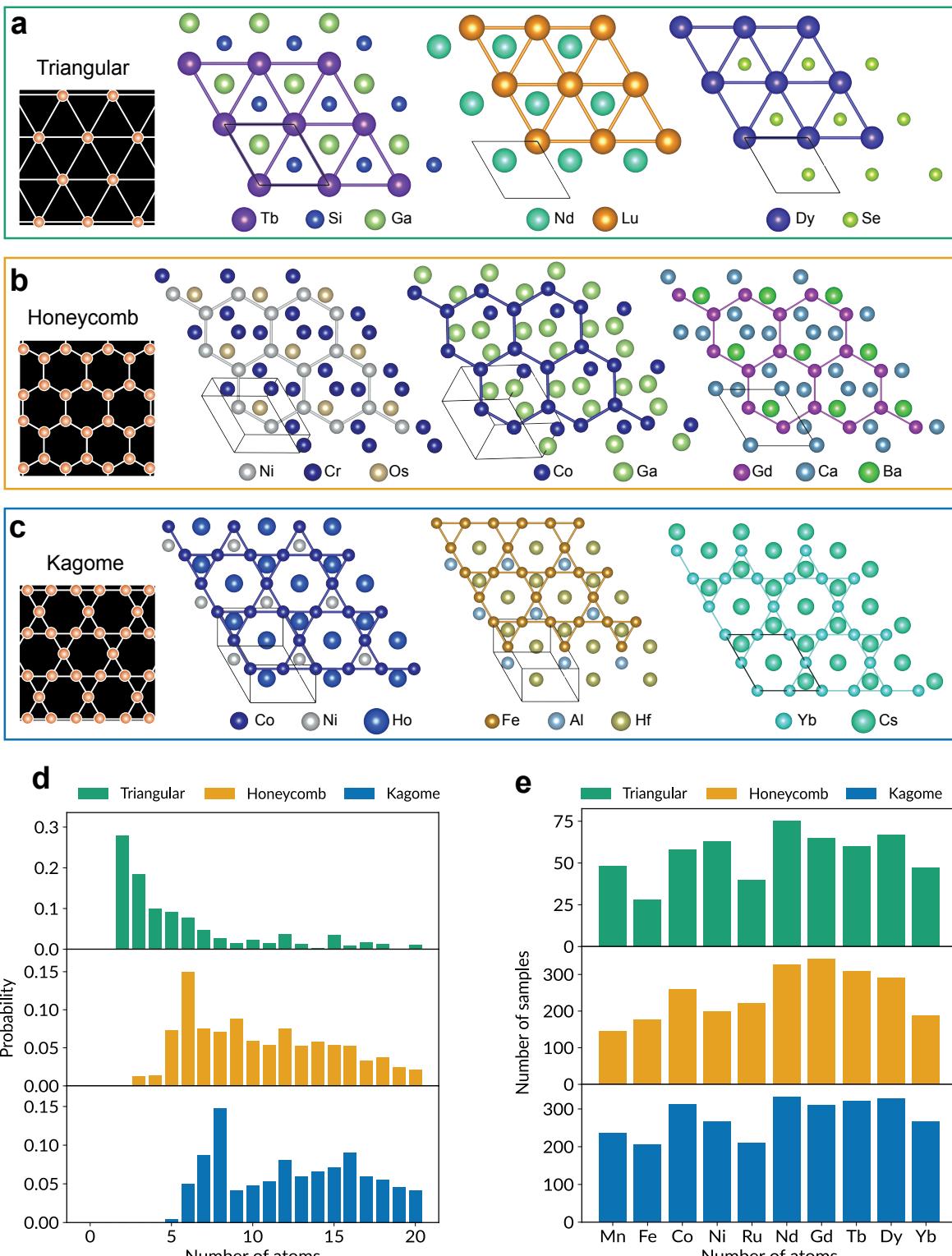


Figure 2. Generated materials with three primary types of archimedean lattices. Archimedean lattice patterns and generated material structures are displayed for **a**. Triangular, **b**. Honeycomb, and **c**. Kagome lattices. **d**. The sampling profile of the number of atoms per unit cell N , generated by measuring the survival ratio from a uniform sampling of N . **e**. The number of materials remaining after pre-screening is presented for the common magnetic atom types in each of the primary geometrical patterns.

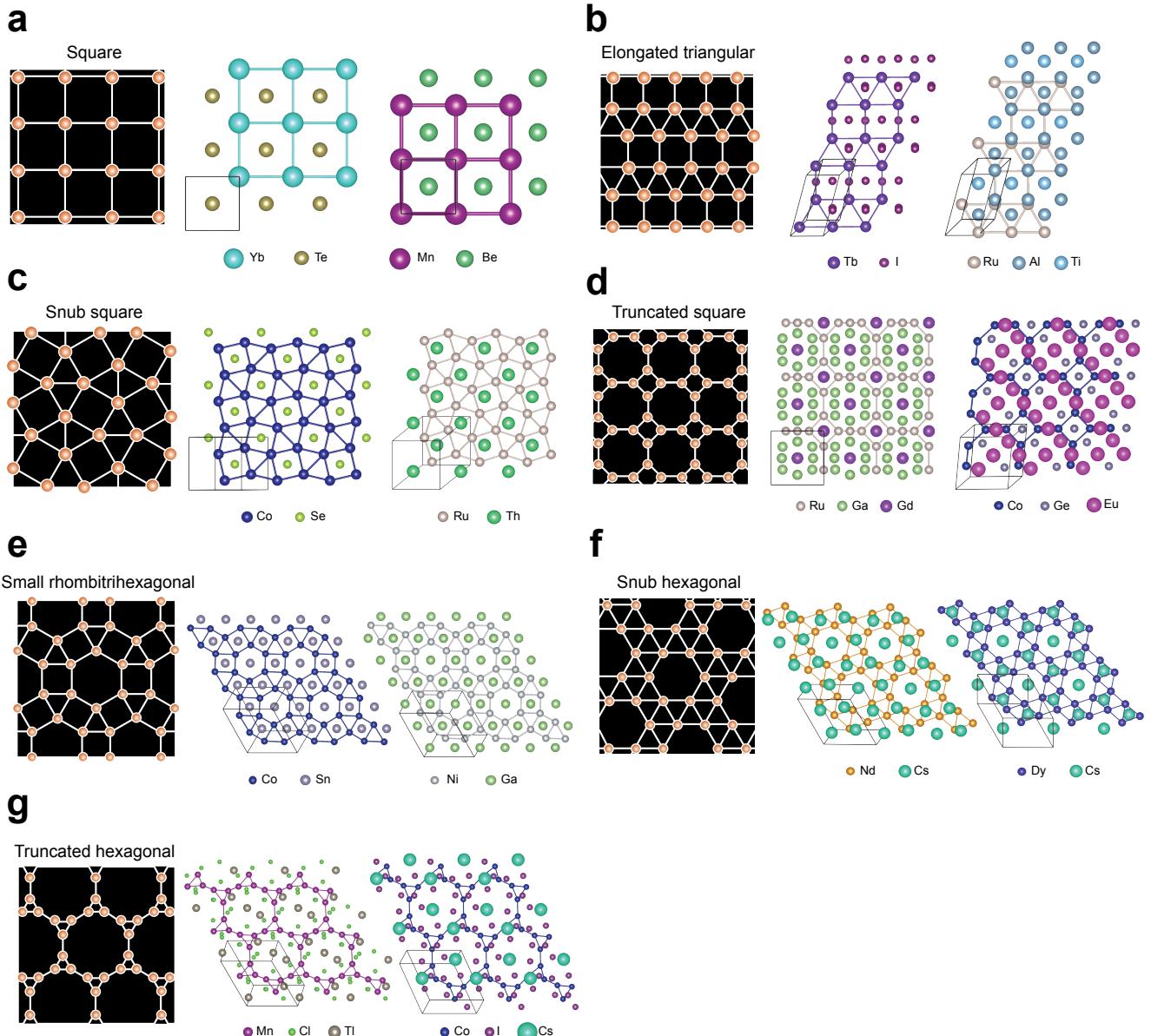


Figure 3. Generated materials with other Archimedean lattice structures. Materials examples covering the rest of Archimedean lattices are presented, with **a**. Square **b**. Elongated triangular **c**. Snub square **d**. Truncated square **e**. Small rhombitrihexagonal **f**. Snub hexagonal **g**. Truncated hexagonal. In each subplot, the AL pattern and two examples of generated materials are displayed.

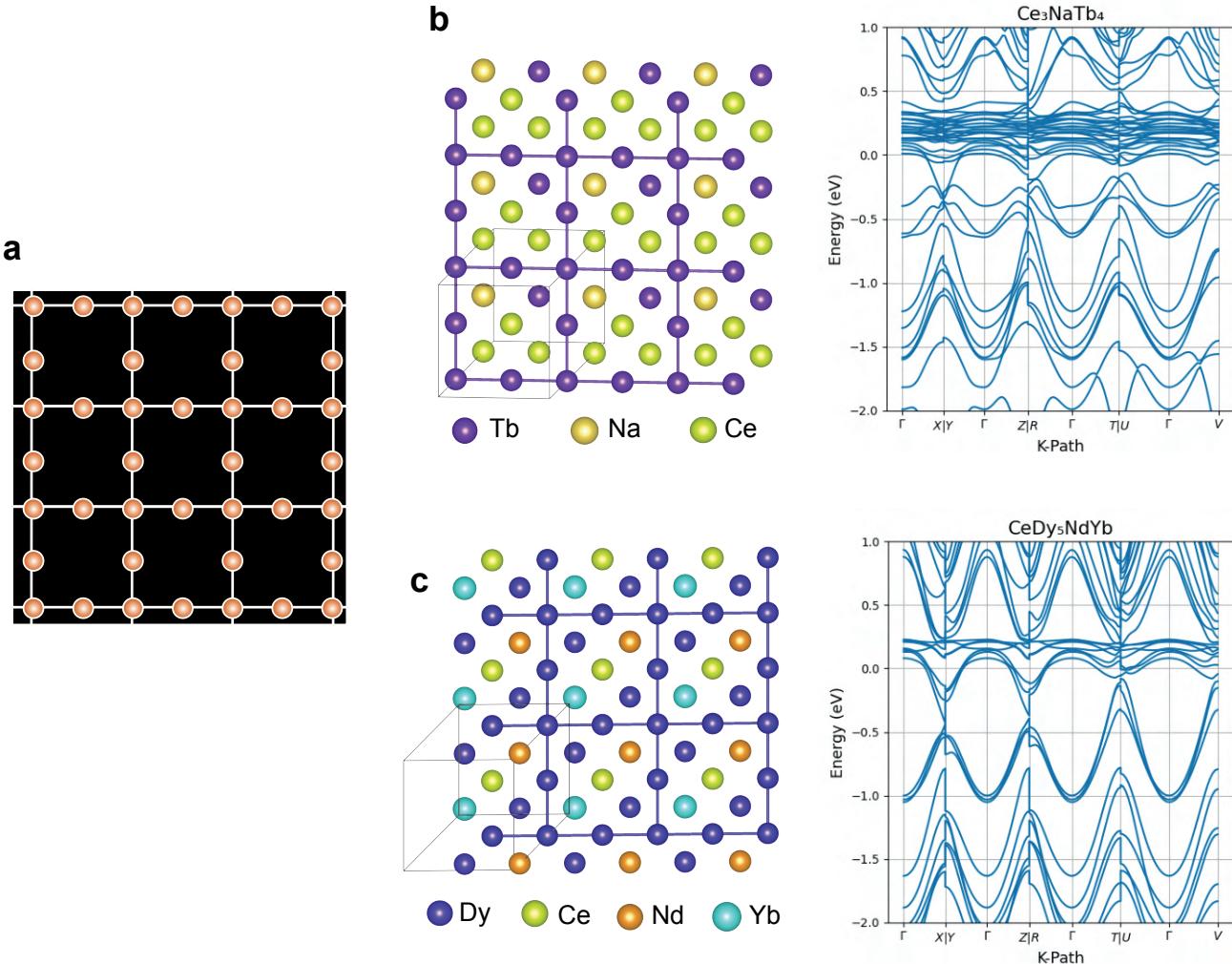


Figure 4. Generated materials of a Lieb-like lattice. **a.** The Lieb lattice pattern that we integrate into the generated structures. The supercell of the Lieb-like lattice materials and the flat band structures of **b.** Ce₃NaTb₄ and **c.** CeDy₃NdYb. We plot the band structures by setting the Fermi level E_F to 0 eV, and the flat bands in both examples are slightly (0.1 – 0.2 eV) above the Fermi level.

Structural Constraint Integration in Generative Model for Discovery of Quantum Material Candidates: Supplementary Information

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Contents

I	Archimedean and Lieb lattices as geometrical pattern constraints	2
II	Initialization of the constraint of structures	5
III	The details of materials generation with geometrical constraint	13
IV	SCIGEN from a probability perspective	15
V	Training of the generative model	17
VI	Stability pre-screening procedures of generated materials	18
VII	Generated materials with Archimedean Lattice constraints	21

I Archimedean and Lieb lattices as geometrical pattern constraints

Archimedean lattices (ALs)^{1,2}, commonly referred to as Archimedean tilings, are distinctive for their planar, uniform tiling, where each vertex configuration is identical. Unlike regular tilings, which utilize only one type of regular polygon, Archimedean lattices incorporate multiple types of regular polygons but are arranged uniformly at each vertex. A key feature of ALs is their vertex-transitivity, which allows any vertex to be mapped to any other through a series of reflections, rotations, and translations, thus preserving the arrangement's overall symmetry.

There are exactly 11 types of ALs, each uniquely defined by the types and sequences of polygons that meet at each vertex. Each AL can be described both as a descriptive name and the numerical name called by the list of the polygons surrounding one vertex. These include the Triangular (3^6), Honeycomb (6^3), and Kagome ($3, 6, 3, 6$) lattices, which are composed of triangles and hexagons in different configurations. The Square lattice (4^4) consists solely of squares. The Elongated triangular ($3^3, 4^2$) and Snub square ($3^2, 4, 3, 4$) lattices mix triangles and squares in varied layouts. Other forms include the Truncated square ($4, 8^2$), Small rhombitrihexagonal ($3, 4, 6, 4$), Snub hexagonal ($3^4, 6$), Truncated hexagonal ($3, 12^2$), and the Great rhombitrihexagonal ($4, 6, 12$), which involve combinations of squares, hexagons, and dodecagons, each offering complex geometric arrangements.

The Lieb lattice is a unique two-dimensional lattice structure characterized by its three sites per unit cell configured in a square shape. The vertices of this lattice are positioned at each corner and at the midpoint of each edge, forming a bipartite lattice. This specific arrangement allows the lattice to be divided into two interpenetrating sublattices, where each site on one only interacts with sites on the other sublattice. The configuration of the Lieb lattice is particularly significant in research areas focusing on optical, magnetic, and transport properties due to its potential for facilitating unusual localized states. These attributes make the Lieb lattice a valuable model in theoretical physics and the practical development of materials with tailored electronic properties.

Table S1 lists the characteristics of Archimedean and Lieb-like lattices. It covers the header that we used for giving file names to each output material, the property of the unit cell, the number of nodes forming AL per unit cell N^c , and the fractional coordinates. Here, we write six lattice parameters as $l_1, l_2, l_3, \alpha, \beta, \gamma$. SCIGEN imposes constraints for the lattice parameters that reflect the AL structures (l_1, l_2, γ), while there are no constraints on the other lattice parameters (l_3, α, β). We also included the constants $k_{latt} = l_1/d^c$ (or l_2/d^c) as the ratio of lattice vector length (l_1, l_2) to the bond length between neighboring vertices (d^c), indicating the relative size of the AL unit cell. Figure S1 visualizes all types of AL and a Lieb-like lattice. The unit cell area is highlighted with blue areas, and the red vertices represent the required positions within the unit cell.

Table S1. Profile of Archimedean lattice and Lieb Lattice

Archimedean lattice	header	Unit cell	N^c	k_{latt}	F_0^c
Triangular (3 ⁶)	tri	Hexagonal ($l_1 = l_2, \gamma = 2\pi/3$)	1	1.0000	(0.0000, 0.0000, z)
Honeycomb (6 ³)	hon	Hexagonal ($l_1 = l_2, \gamma = 2\pi/3$)	2	1.7321	(0.3333, 0.6667, z) (0.6667, 0.3333, z)
Kagome (3, 6, 3, 6)	kag	Hexagonal ($l_1 = l_2, \gamma = 2\pi/3$)	3	2.0000	(0.0000, 0.0000, z) (0.5000, 0.0000, z) (0.0000, 0.5000, z)
Square (4 ⁴)	sqr	Square ($l_1 = l_2, \gamma = \pi/2$)	1	1.0000	(0.0000, 0.0000, z)
Elongated triangular (3 ³ , 4 ²)	elt	Parallelogram ($l_2 = 1.932l_1, \gamma = \pi/3$)	2	1.0000, 1.9319	(0.0000, 0.0000, z) (0.2679, 0.4641, z)
Snub square (3 ² , 4, 3, 4)	sns	Square ($l_1 = l_2, \gamma = \pi/2$)	4	1.9319	(0.3170, 0.1830, z) (0.1830, 0.6830, z) (0.6830, 0.8170, z) (0.8170, 0.3170, z)
Truncated square (4, 8 ²)	tsq	Square ($l_1 = l_2, \gamma = \pi/2$)	4	2.4142	(0.2929, 0.0000, z) (0.7071, 0.0000, z) (0.0000, 0.2929, z) (0.0000, 0.7071, z)
Small rhombitrihexagonal (3, 4, 6, 4)	srh	Hexagonal ($l_1 = l_2, \gamma = 2\pi/3$)	6	2.7321	(0.4226, 0.2113, z) (0.7887, 0.2113, z) (0.7887, 0.5774, z) (0.2113, 0.4226, z) (0.2113, 0.7887, z) (0.5774, 0.7887, z)
Snub hexagonal (3 ⁴ , 6)	snh	Hexagonal ($l_1 = l_2, \gamma = 2\pi/3$)	6	2.6458	(0.4286, 0.1429, z) (0.8571, 0.2857, z) (0.2857, 0.4286, z) (0.7143, 0.5714, z) (0.1429, 0.7143, z) (0.5714, 0.8571, z)
Truncated hexagonal (3, 12 ²)	trh	Hexagonal ($l_1 = l_2, \gamma = 2\pi/3$)	6	3.7321	(0.5774, 0.1547, z) (0.8453, 0.4226, z) (0.5774, 0.4226, z) (0.1547, 0.5774, z) (0.4226, 0.8453, z) (0.4226, 0.5774, z)
Great rhombitrihexagonal (4, 6, 12)	grt	Hexagonal ($l_1 = l_2, \gamma = 2\pi/3$)	12	4.7321	(0.8780, 0.3333, z) (0.8780, 0.5447, z) (0.6667, 0.5447, z) (0.4553, 0.3333, z) (0.4553, 0.1220, z) (0.6667, 0.1220, z) (0.3333, 0.8780, z) (0.5447, 0.8780, z) (0.5447, 0.6667, z) (0.3333, 0.4553, z) (0.1220, 0.4553, z) (0.1220, 0.6667, z)
Lieb	lieb	Square ($l_1 = l_2, \gamma = \pi/2$)	3	2.0000	(0.0000, 0.0000, z) (0.5000, 0.0000, z) (0.0000, 0.5000, z)

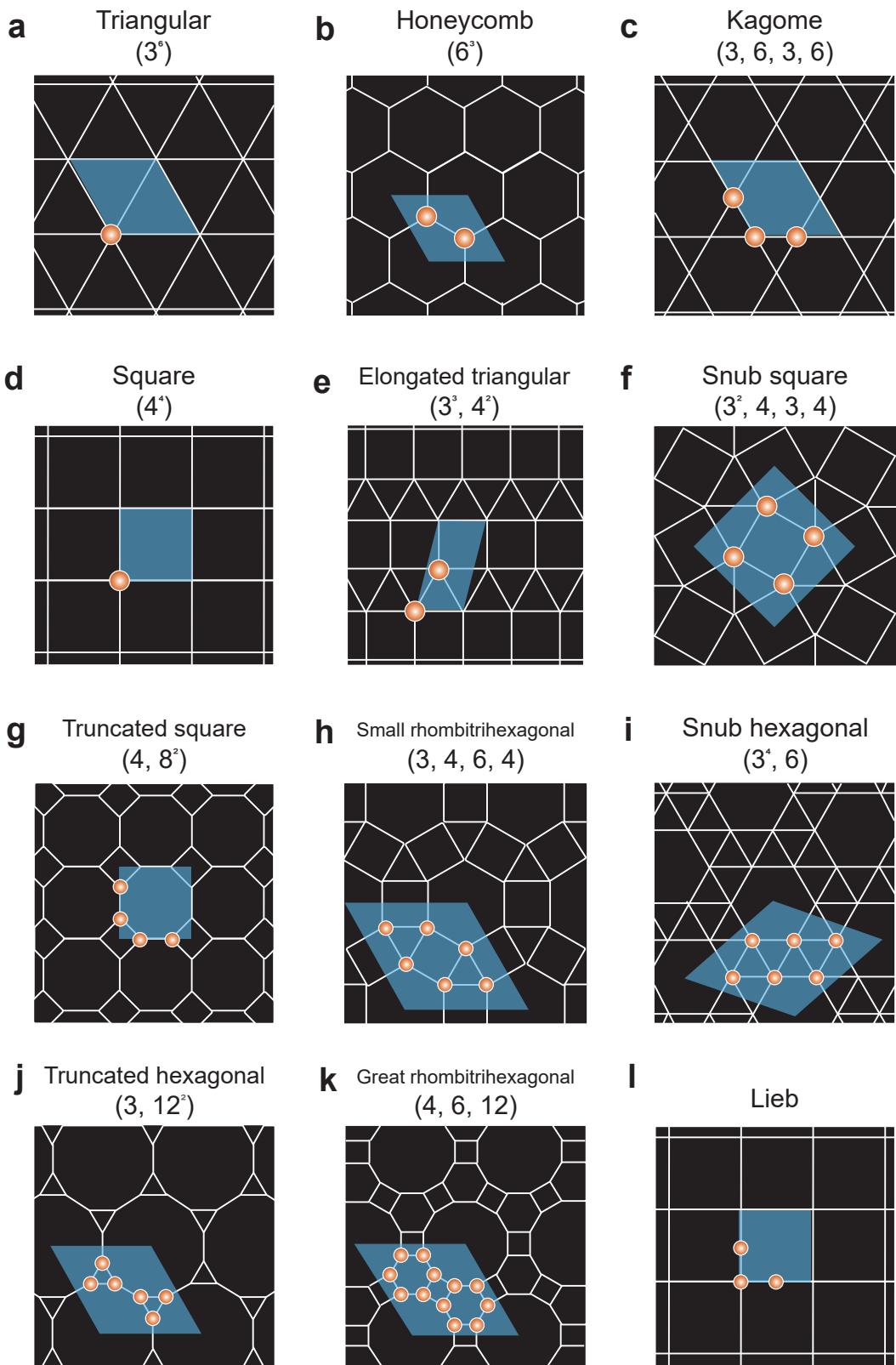


Figure S1. The geometric patterns of Archimedean and Lieb lattices. The geometric pattern is drawn with white lines. The unit cells (blue shaded area) contain nodes (orange dots) for each lattice type. **a.** Triangular **b.** Honeycomb **c.** Kagome **d.** Square **e.** Elongated triangular **f.** Snub square **g.** Truncated square **h.** Small rhombitrihexagonal **i.** Snub hexagonal **j.** Truncated hexagonal **k.** Great rhombitrihexagonal **l.** Lieb lattice.

II Initialization of the constraint of structures

We seek to give constraints to the diffusion model so that the output materials have Archimedean lattice (AL) structures formed with magnetic atoms. Here we present the detailed method of initializing the AL layers, which supplements Fig. 1b of the main article. To begin with, we can arbitrarily choose the AL type we want to impose. In our approach to discovering new materials with unique magnetic characteristics, we aim to place magnetic atoms at the vertices of the AL structures. Specifically, we select ten candidate atoms for these vertices: Mn, Fe, Co, Ni, Ru, Nd, Gd, Tb, Dy, and Yb. Once the vertex atom types \mathcal{A}^c are sampled, their known magnetic properties and electronic configuration affect the coordination environment, which guides the generative process to form stable lattice structures. Next, we consider the bond lengths d^c of vertices within the lattice, which highly depend on the atom type \mathcal{A}^c of the AL vertices. Using CrystalNN³, we identify the bonds of nearest neighbors and then employ kernel density estimation (KDE) to fit the sampled bond lengths, taking into account the metallic radii⁴ of the atoms as the minimum thresholds. Figure S2 illustrates the sampled distribution $p_{d^c}(\mathcal{A}^c)$ of nearest-neighbor distances d^c for each magnetic atom type \mathcal{A}^c , providing a comprehensive overview of the expected bond lengths. The number of atoms per unit cell, denoted as N , is another crucial parameter. We generate a profile of N by sampling from a normal distribution. For each AL and magnetic atom type, we sampled 3000 materials from a uniform distribution with N ranging from $N^c + 1$ to N_{\max} . Here, N^c is the number of vertices forming the unit cell of AL lattices. N_{\max} is the maximum number of atoms per unit cell, and we set it to 20 for profiling the N distribution.

To ensure the generated materials were stable, we apply pre-screening filters to evaluate the reasonableness of the chosen parameters. These filters measure the survival ratios based on charge neutrality, space occupation ratio, and GNN-based classification models. Detailed explanations of the pre-screening procedures are provided in the Methods section and Supplementary Information 5. Figures S3-S6 present $p_N(\mathcal{A}^c)$, the probability distribution of N presenting stable materials with magnetic atom \mathcal{A}^c as AL vertices. Note that $p_N(\mathcal{A}^c)$ is normalized, so that $\sum_N p_N(\mathcal{A}^c) = 1$. By averaging the histogram $p_N(\mathcal{A}^c)$ over all \mathcal{A}^c cases, we build a probability distribution of N as $p_N = \text{mean}_{\mathcal{A}^c}(p_N(\mathcal{A}^c))$. We can sample N from probability distribution p_N , which equally takes all of magnetic atom types \mathcal{A}^c into account. Figure S7 shows p_N as the sampling profile of N for initialization of the generation process. Furthermore, Figure S8 presents the survival ratio of materials for each magnetic atom type as vertices. By rigorously specifying the AL types and sampling the vertex atom types from a uniform distribution, we generate structures with magnetic atoms forming AL structures.

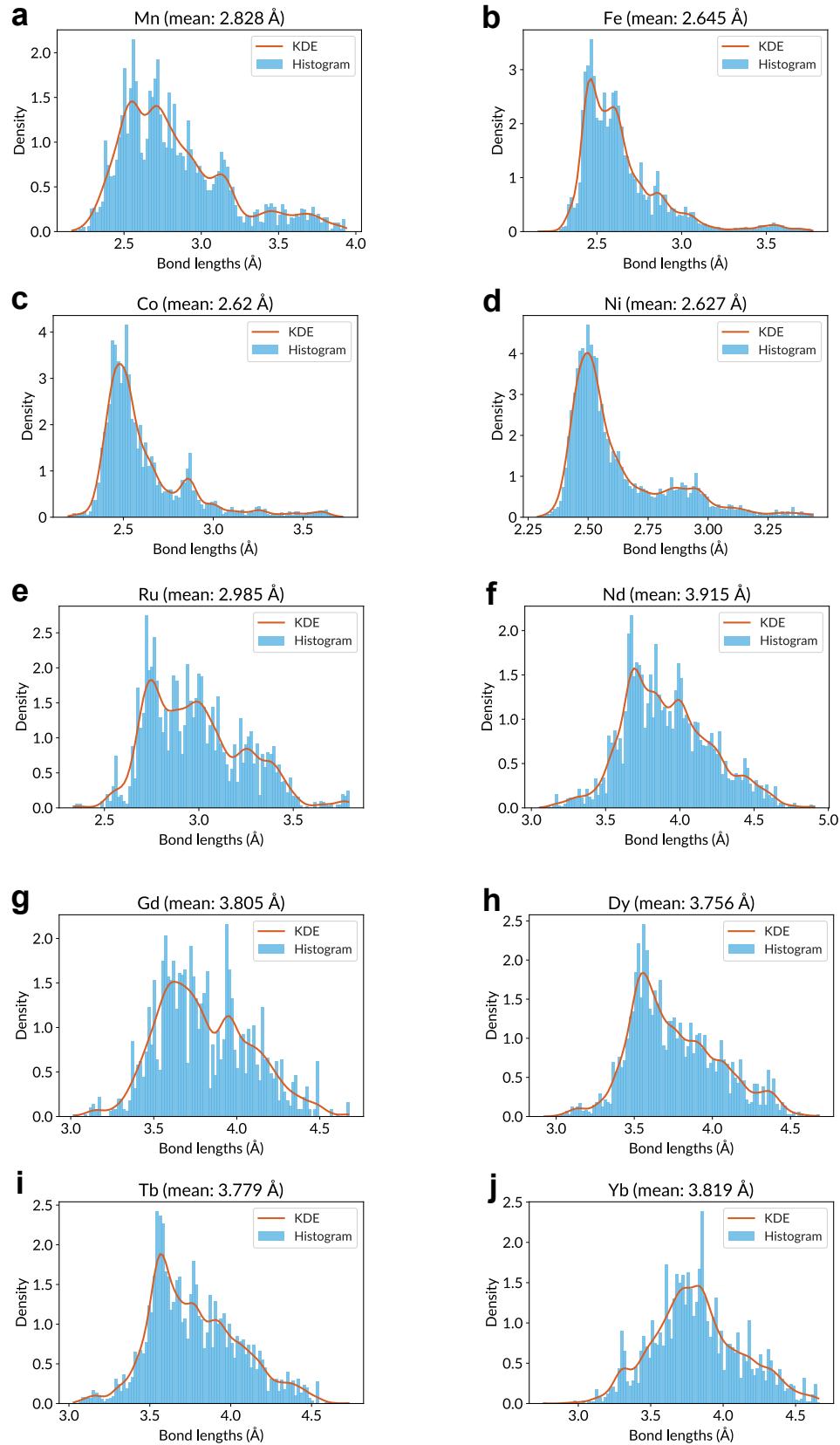


Figure S2. The distribution of bond length $p_{dc}(\mathcal{A}^c)$ sampled from MP-20 dataset. The same atom types located in nearest-neighbor positions are captured, and their distances are measured. The blue histogram (blue) and the red line indicate the sampled distribution and the KDE-fitted curve for **a.** Mn, **b.** Fe, **c.** Co, **d.** Ni, **e.** Ru, **f.** Nd, **g.** Gd, **h.** Tb, **i.** Dy, **j.** Yb.

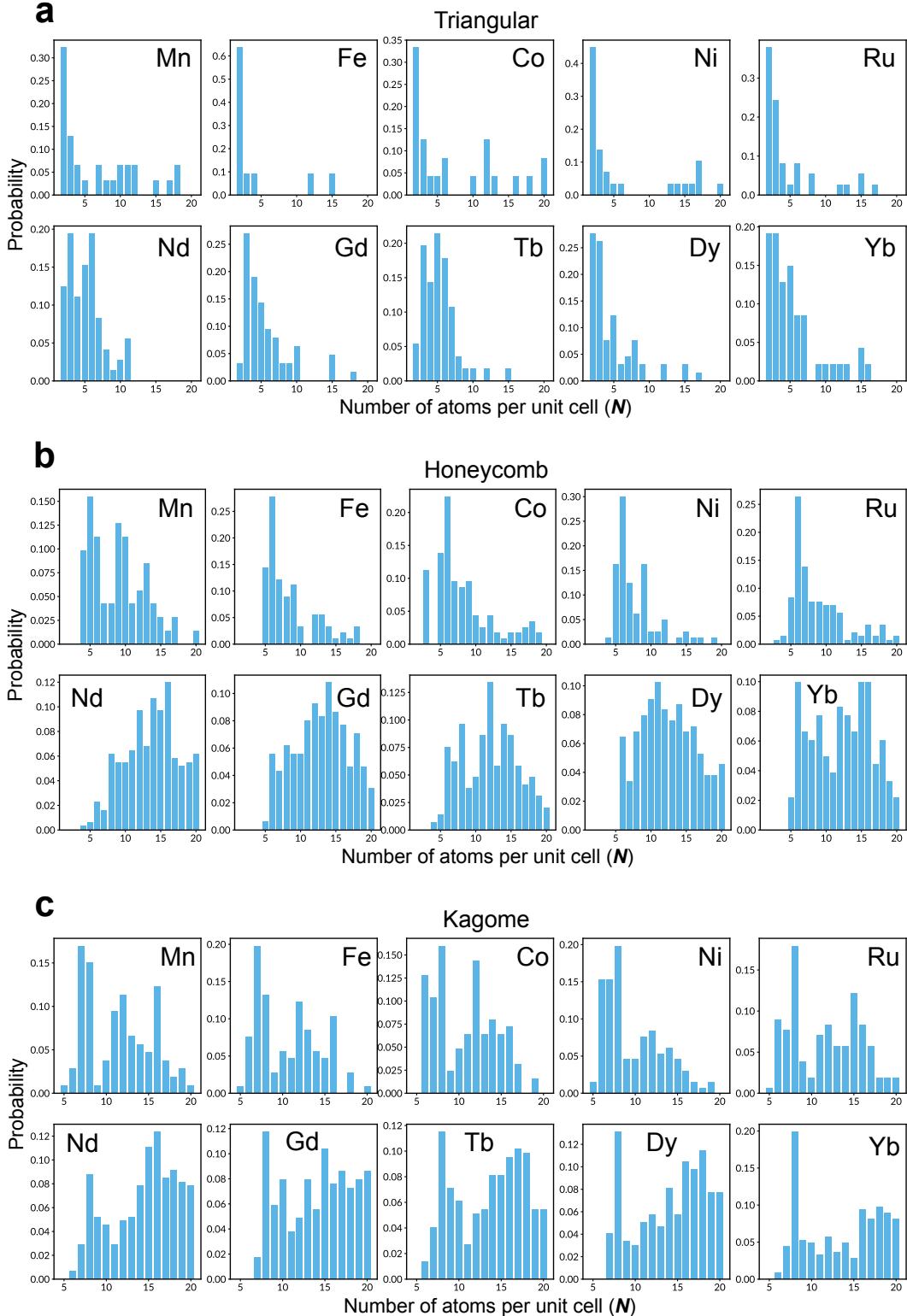


Figure S3. The probability distribution $p_N(\mathcal{A}^c)$ for the number of atoms per unit cell N in case of \mathcal{A}^c as AL vertices. 3000 materials are generated for each type of lattice and each type of magnetic atoms. $N \in [N^c + 1, 20]$ values are sampled from the uniform distribution, and pre-screening filters are applied to evaluate stable materials. **a.** Triangular **b.** Honeycomb **c.** Kagome.

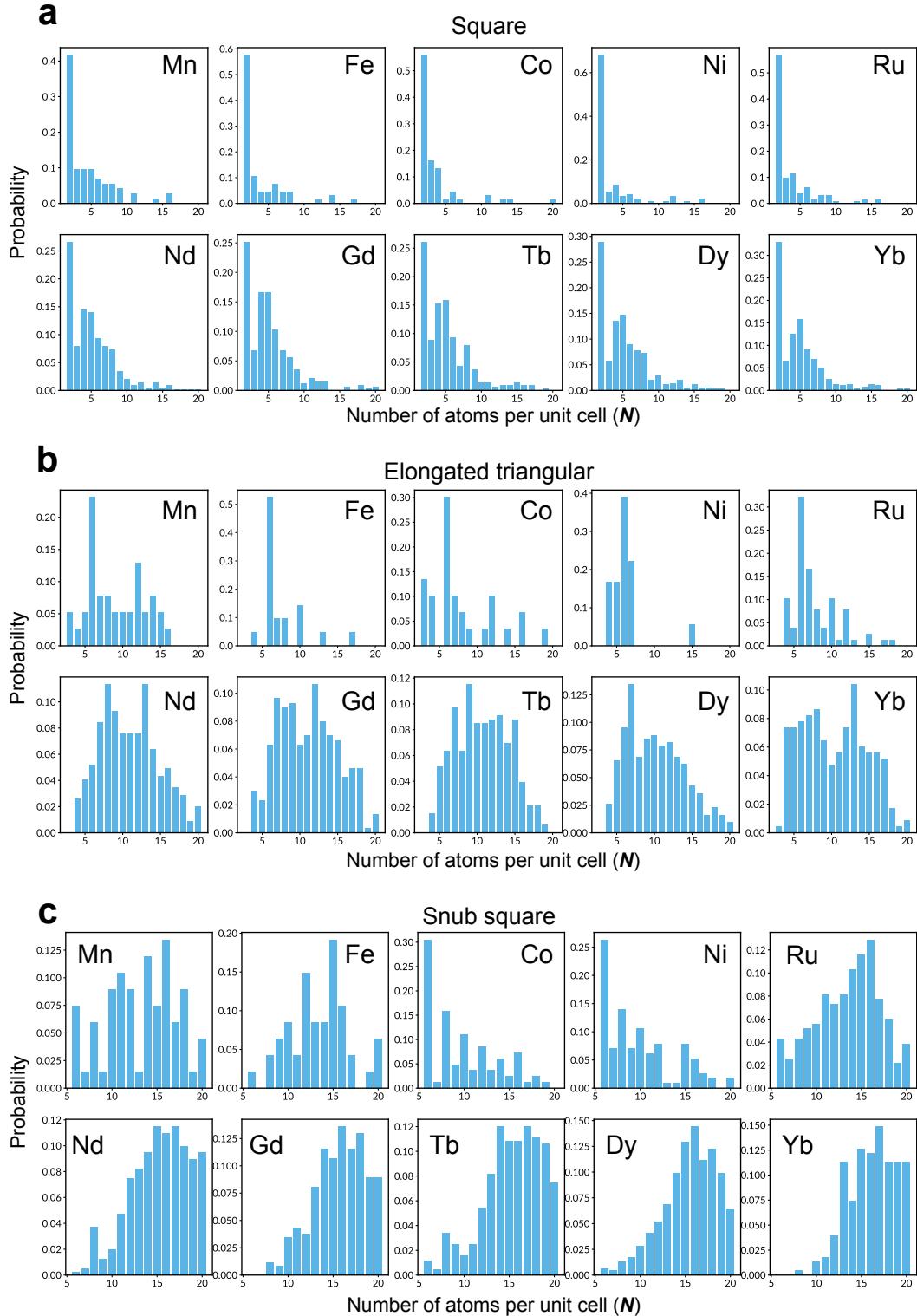


Figure S4. The probability distribution $p_N(\mathcal{A}^c)$ for the number of atoms per unit cell N in case of \mathcal{A}^c as AL vertices. 3000 materials are generated for each type of lattice and each type of magnetic atoms. $N \in [N^c + 1, 20]$ values are sampled from the uniform distribution, and pre-screening filters are applied to evaluate stable materials. **a.** Square **b.** Elongated triangular **c.** Snub square.

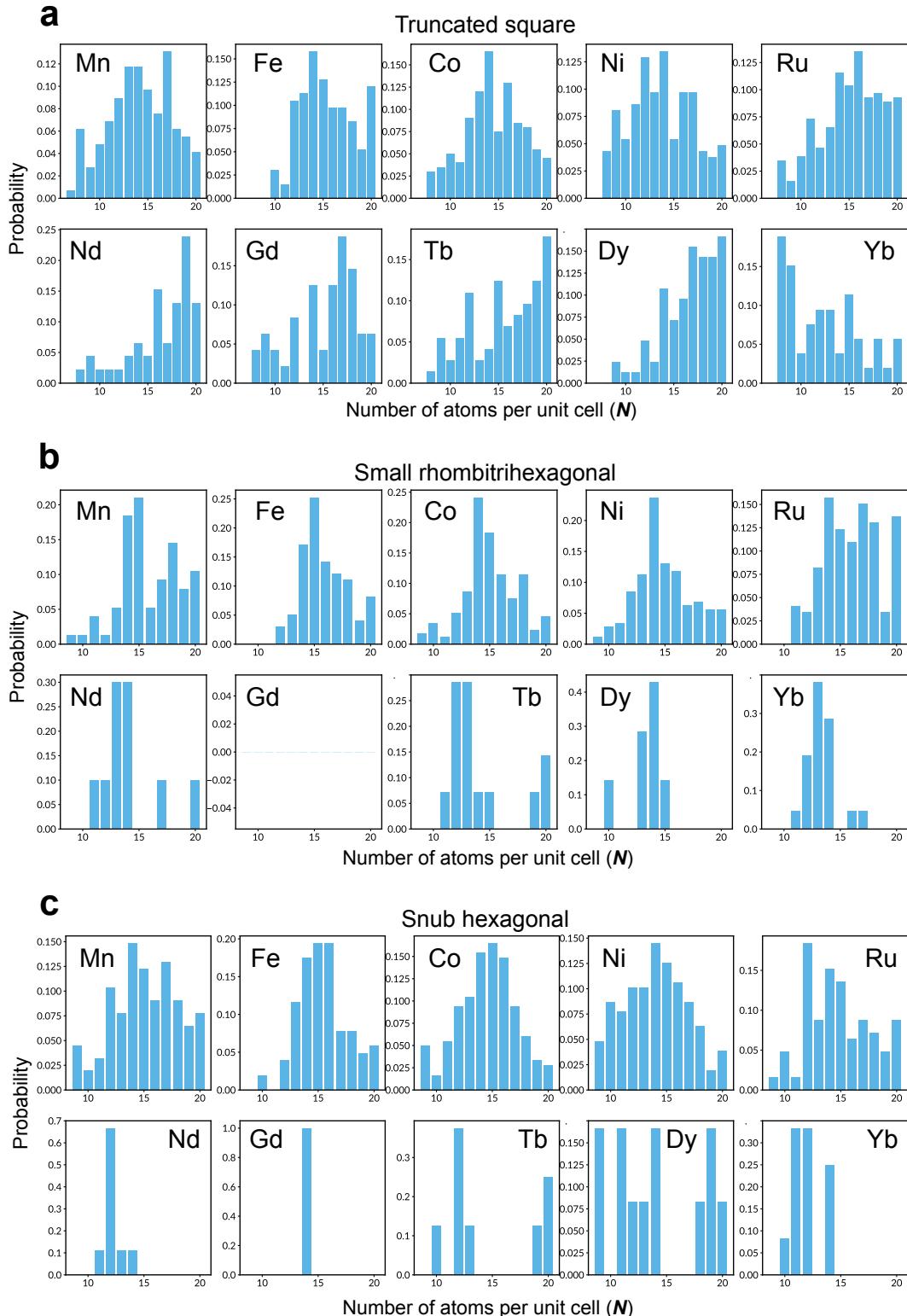


Figure S5. The probability distribution $p_N(\mathcal{A}^c)$ for the number of atoms per unit cell N in case of \mathcal{A}^c as AL vertices. 3000 materials are generated for each type of lattice and each type of magnetic atoms. $N \in [N^c + 1, 20]$ values are sampled from the uniform distribution, and pre-screening filters are applied to evaluate stable materials. **a.** Truncated square **b.** Small rhombitrihexagonal **c.** Snub hexagonal.

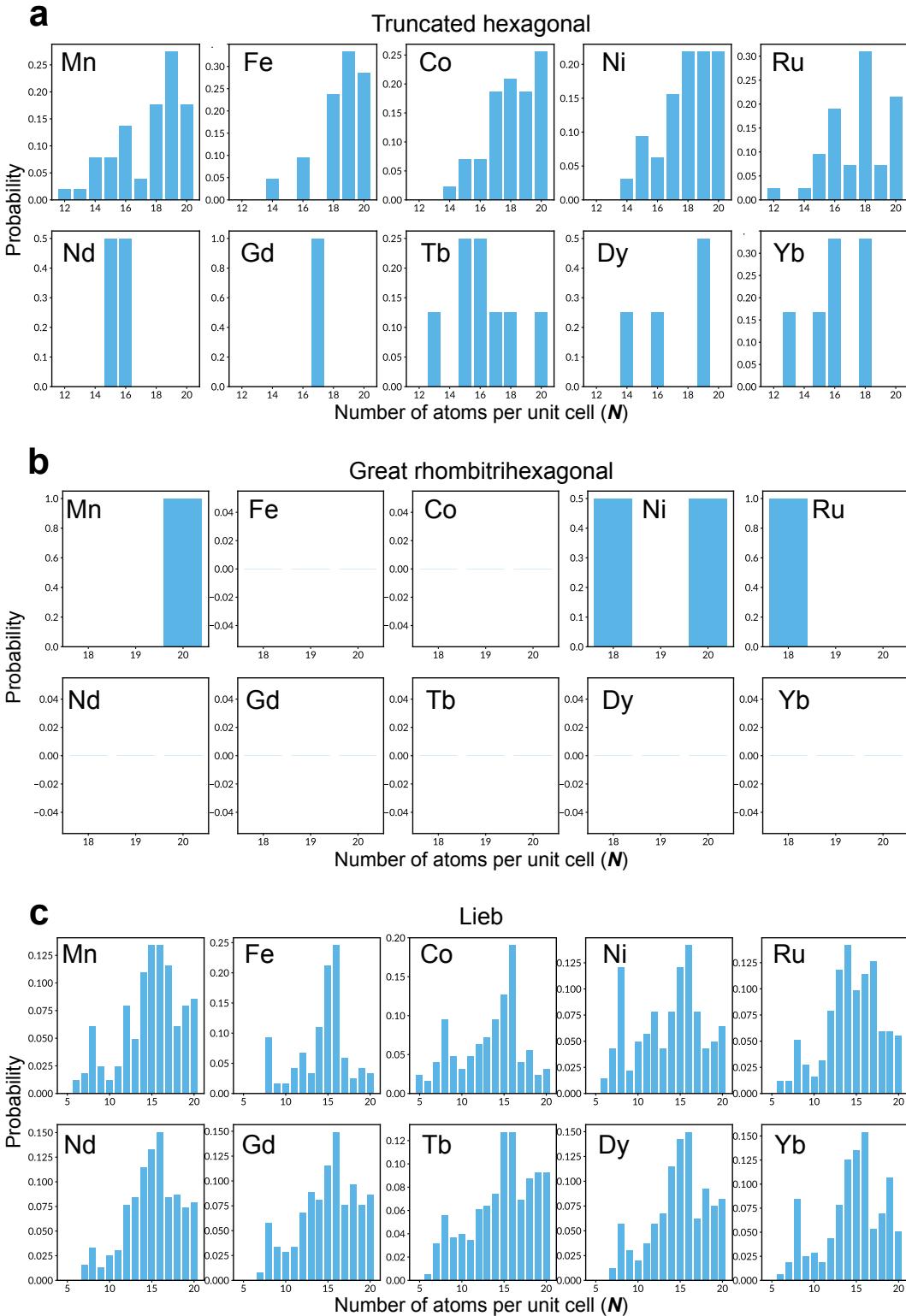


Figure S6. The probability distribution $p_N(\mathcal{A}^c)$ for the number of atoms per unit cell N in case of \mathcal{A}^c as AL vertices. 3000 materials are generated for each type of lattice and each type of magnetic atoms. $N \in [N^c + 1, 20]$ values are sampled from the uniform distribution, and pre-screening filters are applied to evaluate stable materials. **a.** Truncated hexagonal **b.** Great rhombitrihexagonal **c.** Lieb.

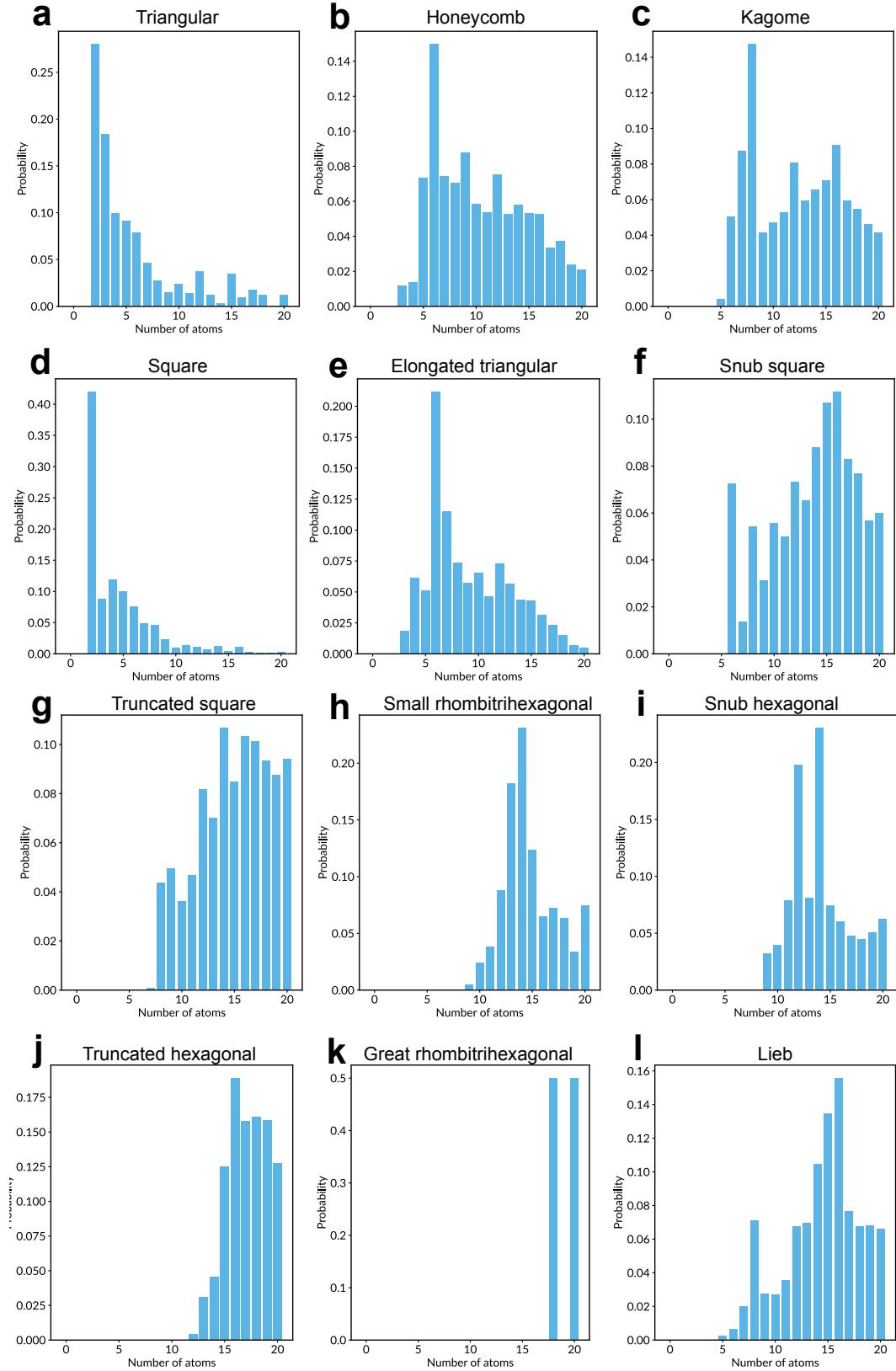


Figure S7. The probability distribution p_N of the number of atoms per unit cell N . The probability distributions $p_N(\mathcal{A}^c)$ are averaged over all magnetic atom types \mathcal{A}^c . **a.** Triangular **b.** Honeycomb **c.** Kagome **d.** Square **e.** Elongated triangular **f.** Snub square **g.** Truncated square **h.** Small rhombitrihexagonal **i.** Snub hexagonal **j.** Truncated hexagonal **k.** Great rhombitrihexagonal **l.** Lieb.

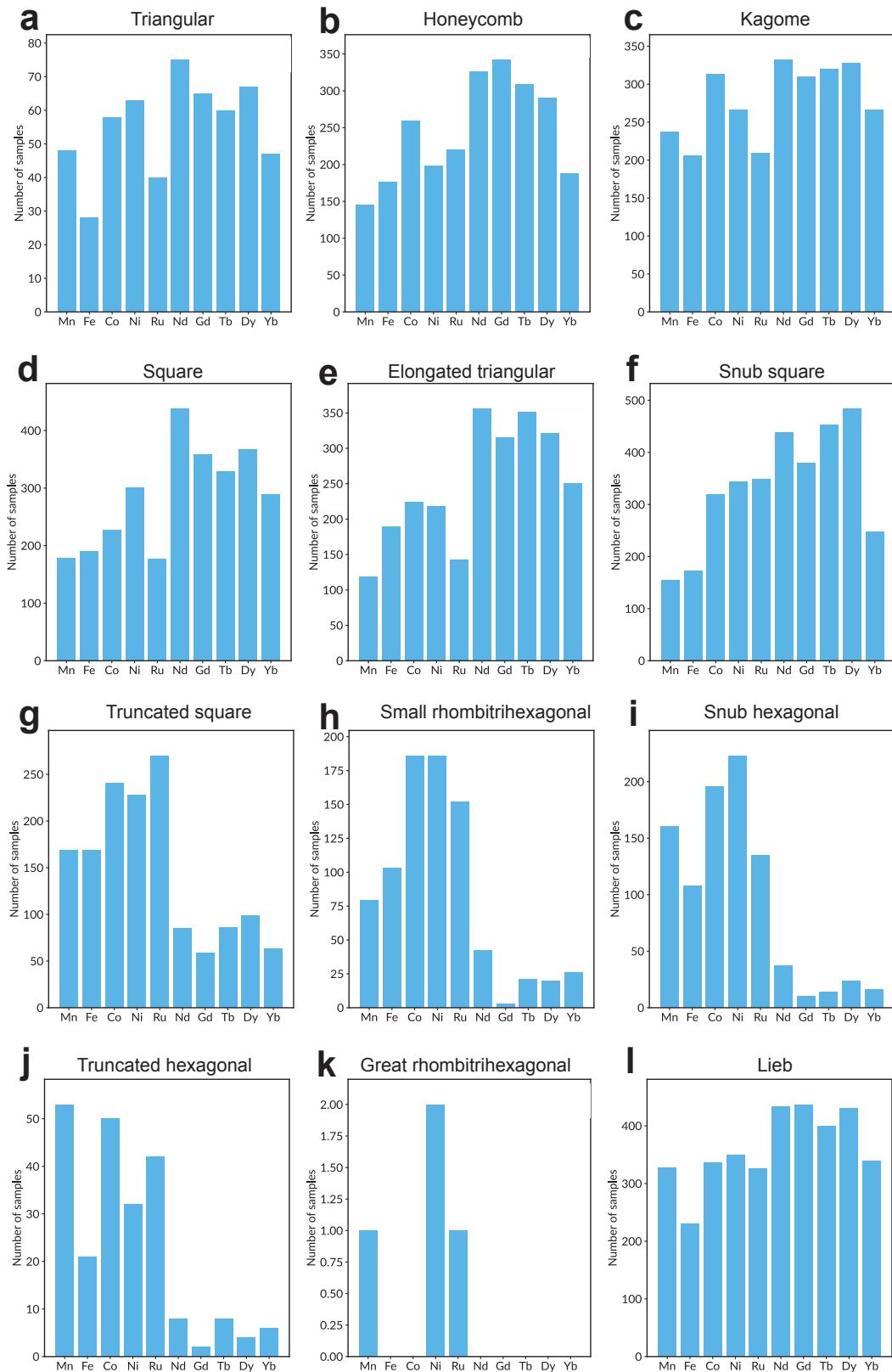


Figure S8. Atom type distribution. The survival ratio was calculated for each of the magnetic atoms forming AL structures. **a.** Triangular **b.** Honeycomb **c.** Kagome **d.** Square **e.** Elongated triangular **f.** Snub square **g.** Truncated square **h.** Small rhombitrihexagonal **i.** Snub hexagonal **j.** Truncated hexagonal **k.** Great rhombitrihexagonal **l.** Lieb

III The details of materials generation with geometrical constraint

Figure 1 in the main manuscript presents the detailed algorithm of our material generation method with structural constraints. Our generative model is implemented based on DiffCSP⁵. Figure S9 elucidates the overview of the denoising method used in this process. Initially, we input the structure $\mathbf{M}_t^u = (\mathbf{L}_t, \mathbf{F}_t, \mathbf{A}_t)$, where each component is denoised to become $\mathbf{M}_{t-1}^u = (\mathbf{L}_{t-1}^u, \mathbf{F}_{t-1}^u, \mathbf{A}_{t-1}^u)$. This transformation is achieved by predicting the denoising terms $\hat{\epsilon}_L$, $\hat{\epsilon}_F$, and $\hat{\epsilon}_A$.

Figure S10 illustrates the procedure to integrate the constrained structure with the unconstrained components to guide the material generation forming AL structures. For each timestamp t of the denoising process, whenever we have \mathbf{M}_t^u , we obtain \mathbf{M}_t by guiding the structure with the constrained component \mathbf{M}_t^c . The constrained structure is represented as $\mathbf{M}_t^c = (\mathbf{L}_t^c, \mathbf{F}_t^c, \mathbf{A}_t^c)$, and the unconstrained structure is $\mathbf{M}_t^u = (\mathbf{L}_t^u, \mathbf{F}_t^u, \mathbf{A}_t^u)$. We utilize masks to distinguish between the constrained and unconstrained parts of the structure. The first N^c atoms are the constrained atoms and the other atoms are unconstrained. The mask for lattice, coordinates, and atom types are \mathbf{m}_L , \mathbf{m}_F and \mathbf{m}_A respectively. These masks are equal to 1 for the constrained components, which we aim to impose on the generated materials. In SCIGEN, \mathbf{m}_L is 1 for the \mathbf{l}_1 and \mathbf{l}_2 , as these two lattice vectors define the unit cell of AL layer and they need to result in the lattice vectors we impose. On the other hand, \mathbf{m}_L is equal to 0 for \mathbf{l}_3 , as \mathbf{l}_3 does not involve in the formation of AL structure directly and we can let the model to generate \mathbf{l}_3 . For fractional coordinates, \mathbf{m}_F is equal to 1 for the atoms indexed from first to N^c -th atoms, which form AL layer structures. The same rule applies for \mathbf{m}_A , the mask for atom types.

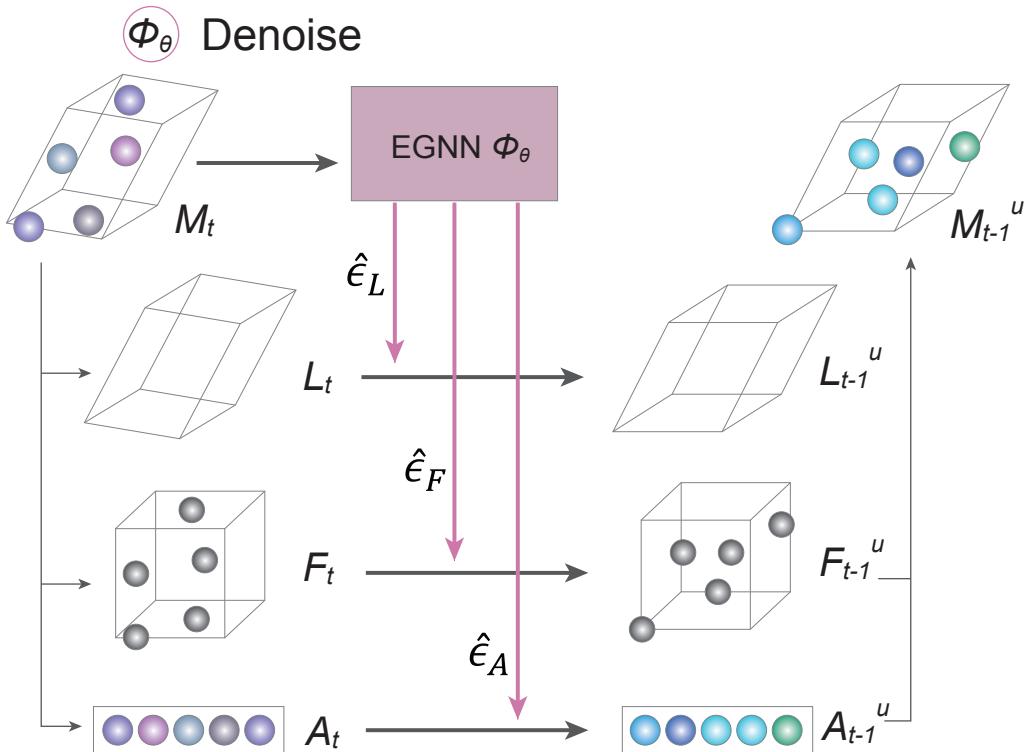


Figure S9. Method of generative model for denoising material. We apply the denoising term prediction implemented in DiffCSP. We input a diffused crystal structure \mathbf{M}_t^u to get the denoising term for the lattice, the fractional coordinates, and the atom type.

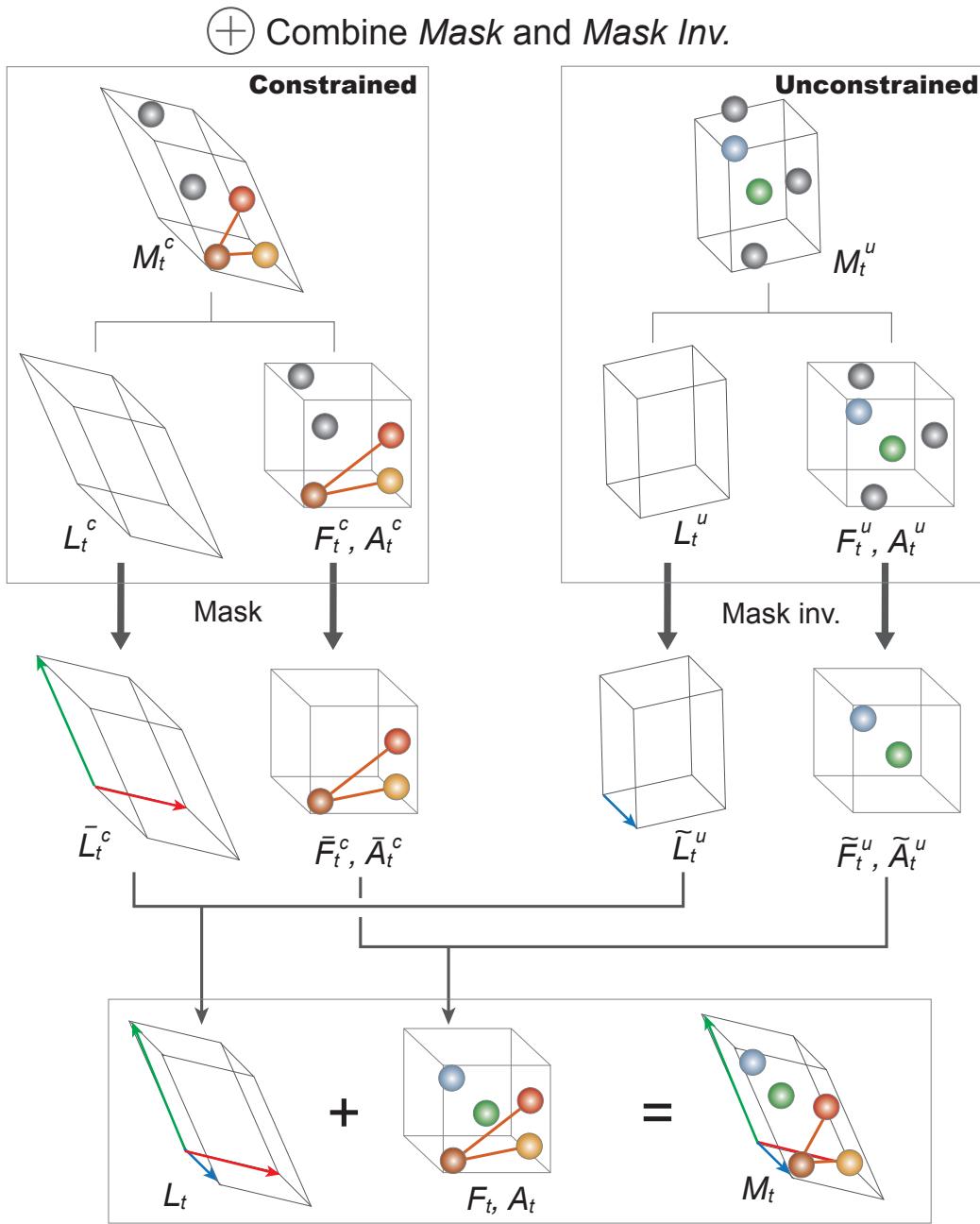


Figure S10. Method of generative model for denoising material. Both the constrained structures M_t^c and unconstrained ones M_t^u are decomposed to the lattice, atom types, and coordinates. After applying the masks to select the components to care for, structural components are integrated.

IV SCIGEN from a probability perspective

By design, because of the masking mechanics of SCIGEN, given the constrained structure \mathbf{M}_0^c , the generated structure \mathbf{M}_0 would have $\mathbf{m} \odot \mathbf{M}_0 = \mathbf{m} \odot \mathbf{M}_0^c$. However, for the scheme to be useful, the distribution of the generated structure $P(\mathbf{M}_0|\mathbf{M}_0^c)$ needs to reflect the actual distribution of the stable material conditional on the constraints imposed. Let's assume that the trained model has q as its diffusion inference model, and p as its denoising generative model. For a given constrained structure \mathbf{M}_0^c , we can independently sample diffused constrained structure at every time step with

$$P(\mathbf{M}_t^c|\mathbf{M}_0^c) = q_{0,t}(\mathbf{M}_t^c|\mathbf{M}_0^c).$$

For compactness, let's define $\bar{\mathbf{M}}$ as the masked part of \mathbf{M} , $\mathbf{m} \odot \mathbf{M}$, and $\tilde{\mathbf{M}}$ as the unmasked part of \mathbf{M} , $(1 - \mathbf{m}) \odot \mathbf{M}$. This means that

$$\begin{aligned}\mathbf{M}_t^c &= \bar{\mathbf{M}}_t^c + \tilde{\mathbf{M}}_t^c \\ \mathbf{M}_t^u &= \bar{\mathbf{M}}_t^u + \tilde{\mathbf{M}}_t^u \\ \mathbf{M}_t &= \bar{\mathbf{M}}_t^c + \tilde{\mathbf{M}}_t^u\end{aligned}$$

Then, consider a generation of a structure \mathbf{M}_0 given \mathbf{M}_t^c for every time step $t \in [0..T]$, $\mathbf{M}_{0:T}^c$, the distribution of \mathbf{M}_0 is

$$\begin{aligned}P(\mathbf{M}_0|\mathbf{M}_{0:T}^c) &= P(\bar{\mathbf{M}}_0^c, \tilde{\mathbf{M}}_0^u|\bar{\mathbf{M}}_{0:T}^c, \tilde{\mathbf{M}}_{0:T}^c) \\ &= P(\tilde{\mathbf{M}}_0^u|\bar{\mathbf{M}}_{0:T}^c, \tilde{\mathbf{M}}_{0:T}^c) \\ &= \int P(\bar{\mathbf{M}}_0^u, \tilde{\mathbf{M}}_0^u|\bar{\mathbf{M}}_{0:T}^c, \tilde{\mathbf{M}}_{0:T}^c)d\bar{\mathbf{M}}_0^u \\ &= \int p_{1,0}(\bar{\mathbf{M}}_0^u, \tilde{\mathbf{M}}_0^u|\bar{\mathbf{M}}_1^c, \tilde{\mathbf{M}}_1^u) \cdot P(\bar{\mathbf{M}}_1^c, \tilde{\mathbf{M}}_1^u|\bar{\mathbf{M}}_{0:T}^c, \tilde{\mathbf{M}}_{0:T}^c)d\bar{\mathbf{M}}_0^ud\tilde{\mathbf{M}}_1^u \\ &= \int p_{1,0}(\bar{\mathbf{M}}_0^u, \tilde{\mathbf{M}}_0^u|\bar{\mathbf{M}}_1^c, \tilde{\mathbf{M}}_1^u) \cdot P(\tilde{\mathbf{M}}_1^u|\bar{\mathbf{M}}_{0:T}^c, \tilde{\mathbf{M}}_{0:T}^c)d\bar{\mathbf{M}}_0^ud\tilde{\mathbf{M}}_1^u \\ &\dots \\ &= \int \left[\prod_{t=1}^T p_{t,t-1}(\bar{\mathbf{M}}_{t-1}^u, \tilde{\mathbf{M}}_{t-1}^u|\bar{\mathbf{M}}_t^c, \tilde{\mathbf{M}}_t^u) \right] \cdot P(\tilde{\mathbf{M}}_T^u|\bar{\mathbf{M}}_{0:T}^c, \tilde{\mathbf{M}}_{0:T}^c)d\bar{\mathbf{M}}_{0:T-1}^ud\tilde{\mathbf{M}}_{1:T}^u \\ &= \int \left[\prod_{t=1}^T p_{t,t-1}(\bar{\mathbf{M}}_{t-1}^u, \tilde{\mathbf{M}}_{t-1}^u|\bar{\mathbf{M}}_t^c, \tilde{\mathbf{M}}_t^u) \right] \cdot P(\tilde{\mathbf{M}}_T^u)d\bar{\mathbf{M}}_{0:T-1}^ud\tilde{\mathbf{M}}_{1:T}^u \\ &= \int p_{1:T,0:T-1}(\bar{\mathbf{M}}_{0:T-1}^u, \tilde{\mathbf{M}}_{0:T}^u|\bar{\mathbf{M}}_{1:T}^c)d\bar{\mathbf{M}}_{0:T-1}^ud\tilde{\mathbf{M}}_{1:T}^u \\ &= p_{1:T,0}(\tilde{\mathbf{M}}_0^u|\bar{\mathbf{M}}_{1:T}^c).\end{aligned}$$

The fourth equality is from the Markov structure of the generative model. The sixth equality is from recursively applying second to fifth equalities. Since \mathbf{M}_T^u was randomly sampled, it is independent of $\mathbf{M}_{0:T}^c$. Hence, the seventh equality holds. Then, the Markov structure gives the eighth equality, and marginal integration gives the last. However, this result is for a specific sequence $\mathbf{M}_{0:T}^c$. By taking average over $\mathbf{M}_{1:T}^c$ for a given constrained structure \mathbf{M}_0^c ,

$$\begin{aligned}P(\mathbf{M}_0|\mathbf{M}_0^c) &= \int p_{1:T,0}(\tilde{\mathbf{M}}_0^u|\bar{\mathbf{M}}_{1:T}^c) \cdot q_{0,1:T}(\mathbf{M}_{1:T}^c|\mathbf{M}_0^c)d\mathbf{M}_{1:T}^c \\ &= \int p_{1:T,0}(\tilde{\mathbf{M}}_0^u|\bar{\mathbf{M}}_{1:T}^c) \cdot q_{0,1:T}(\bar{\mathbf{M}}_{1:T}^c|\mathbf{M}_0^c)d\bar{\mathbf{M}}_{1:T}^c \\ &\approx q_{0,0}(\tilde{\mathbf{M}}_0^u|\bar{\mathbf{M}}_0^c)\end{aligned}$$

where the approximation holds if p from the underlying generative model is well-trained, so that p can approximate the diffusion pathway of q in a reverse order. This implies that the SCIGEN structure generation given \mathbf{M}_0^c is equivalent to conditional generation of the underlying generative model by constraining $\bar{\mathbf{M}}_0$ with $\bar{\mathbf{M}}_0^c$ and filling in $\tilde{\mathbf{M}}_0$.

One might also ask whether this result would still hold when the base model contains predictor-corrector mechanism like in DiffCSP used in our demonstration since the prediction at half-time-step points require additional masking from diffused

constrained structure. Similar to above, but we also given \mathbf{M}_t^c for every half-time step $t \in [\frac{1}{2}..T - \frac{1}{2}]$, i.e., given $\mathbf{M}_{0:\frac{1}{2}:T}^c$,

$$\begin{aligned}
P(\mathbf{M}_0 | \mathbf{M}_{0:\frac{1}{2}:T}^c) &= P(\mathbf{L}_0, \mathbf{F}_0, \mathbf{A}_0 | \mathbf{M}_{0:\frac{1}{2}:T}^c) \\
&= P(\mathbf{L}_0, \bar{\mathbf{F}}_0^c, \tilde{\mathbf{F}}_0^u, \mathbf{A}_0 | \mathbf{M}_{0:\frac{1}{2}:T}^c) \\
&= P(\mathbf{L}_0, \tilde{\mathbf{F}}_0^u, \mathbf{A}_0 | \mathbf{M}_{0:\frac{1}{2}:T}^c) \\
&= \int P(\mathbf{L}_0, \mathbf{F}_0^u, \mathbf{A}_0 | \mathbf{M}_{0:\frac{1}{2}:T}^c) d\bar{\mathbf{F}}_0^u \\
&= \int p_{1,0}^{\mathbf{F},c}(\mathbf{F}_0^u | \mathbf{L}_0, \mathbf{F}_{\frac{1}{2}}, \mathbf{A}_0) P(\mathbf{L}_0, \mathbf{F}_{\frac{1}{2}}, \mathbf{A}_0 | \mathbf{M}_{0:\frac{1}{2}:T}^c) d\bar{\mathbf{F}}_0^u d\tilde{\mathbf{F}}_{\frac{1}{2}}^u \\
&= \int p_{1,0}^{\mathbf{F},c}(\mathbf{F}_0^u | \mathbf{L}_0, \mathbf{F}_{\frac{1}{2}}, \mathbf{A}_0) P(\mathbf{L}_0, \tilde{\mathbf{F}}_{\frac{1}{2}}^u, \mathbf{A}_0 | \mathbf{M}_{0:\frac{1}{2}:T}^c) d\bar{\mathbf{F}}_0^u d\tilde{\mathbf{F}}_{\frac{1}{2}}^u \\
&= \int p_{1,0}^{\mathbf{F},c}(\mathbf{F}_0^u | \mathbf{L}_0, \mathbf{F}_{\frac{1}{2}}, \mathbf{A}_0) P(\mathbf{L}_0, \mathbf{F}_{\frac{1}{2}}^u, \mathbf{A}_0 | \mathbf{M}_{0:\frac{1}{2}:T}^c) d\bar{\mathbf{F}}_0^u d\bar{\mathbf{F}}_{\frac{1}{2}}^u d\tilde{\mathbf{F}}_{\frac{1}{2}}^u \\
&= \int p_{1,0}^{\mathbf{F},c}(\mathbf{F}_0^u | \mathbf{L}_0, \mathbf{F}_{\frac{1}{2}}, \mathbf{A}_0) P(\tilde{\mathbf{L}}_0^u, \mathbf{F}_{\frac{1}{2}}^u, \tilde{\mathbf{A}}_0 | \mathbf{M}_{0:\frac{1}{2}:T}^c) d\bar{\mathbf{F}}_0^u d\mathbf{F}_{\frac{1}{2}}^u \\
&= \int p_{1,0}^{\mathbf{F},c}(\mathbf{F}_0^u | \mathbf{L}_0, \mathbf{F}_{\frac{1}{2}}, \mathbf{A}_0) P(\mathbf{L}_0^u, \mathbf{F}_{\frac{1}{2}}^u, \mathbf{A}_0^u | \mathbf{M}_{0:\frac{1}{2}:T}^c) d\bar{\mathbf{M}}_0^u d\mathbf{F}_{\frac{1}{2}}^u \\
&= \int p_{1,0}^{\mathbf{F},c}(\mathbf{F}_0^u | \mathbf{L}_0, \mathbf{F}_{\frac{1}{2}}, \mathbf{A}_0) p_{1,0}^{\mathbf{L}}(\mathbf{L}_0^u | \mathbf{M}_1) p_{1,0}^{\mathbf{F},p}(\mathbf{F}_{\frac{1}{2}}^u | \mathbf{M}_1) p_{1,0}^{\mathbf{A}}(\mathbf{A}_0^u | \mathbf{M}_1) P(\mathbf{M}_1 | \mathbf{M}_{0:\frac{1}{2}:T}^c) d\bar{\mathbf{M}}_0^u d\mathbf{F}_{\frac{1}{2}}^u d\tilde{\mathbf{M}}_1^u
\end{aligned}$$

where fifth, and last equality are from corrector, and predictor mechanisms, respectively. We can combine the product of the first four terms as $p_{1,0}(\mathbf{L}_0^u, \mathbf{F}_0^u, \mathbf{A}_0^u, \mathbf{F}_{\frac{1}{2}}^u | \bar{\mathbf{L}}_0^c, \bar{\mathbf{A}}_0^c, \bar{\mathbf{F}}_{\frac{1}{2}}^c, \mathbf{M}_1) = p_{1,0}(\mathbf{M}_0^u, \mathbf{F}_{\frac{1}{2}}^u | \bar{\mathbf{L}}_0^c, \bar{\mathbf{A}}_0^c, \bar{\mathbf{F}}_{\frac{1}{2}}^c, \mathbf{M}_1)$. We can apply this recursively:

$$\begin{aligned}
P(\mathbf{M}_0 | \mathbf{M}_{0:\frac{1}{2}:T}^c) &= \int \prod_{t=0}^{T-1} \left[p_{t+1,t}(\mathbf{M}_t^u, \mathbf{F}_{t+\frac{1}{2}}^u | \bar{\mathbf{L}}_t^c, \bar{\mathbf{A}}_t^c, \bar{\mathbf{F}}_{t+\frac{1}{2}}^c, \mathbf{M}_{t+1}) \right] \cdot P(\mathbf{M}_T | \mathbf{M}_{0:\frac{1}{2}:T}^c) d\bar{\mathbf{M}}_0^u d\mathbf{F}_{\frac{1}{2}:T-\frac{1}{2}}^u d\tilde{\mathbf{M}}_{1:T}^u \\
&= \int \prod_{t=0}^{T-1} \left[p_{t+1,t}(\mathbf{M}_t^u, \mathbf{F}_{t+\frac{1}{2}}^u | \bar{\mathbf{L}}_t^c, \bar{\mathbf{A}}_t^c, \bar{\mathbf{F}}_{t+\frac{1}{2}}^c, \mathbf{M}_{t+1}) \right] \cdot P(\tilde{\mathbf{M}}_T^u) d\bar{\mathbf{M}}_0^u d\mathbf{F}_{\frac{1}{2}:T-\frac{1}{2}}^u d\tilde{\mathbf{M}}_{1:T}^u \\
&= \int p_{1:T,0:T-1}(\mathbf{M}_{0:T-1}^u, \mathbf{F}_{\frac{1}{2},T-\frac{1}{2}}^u | \bar{\mathbf{L}}_0^c, \bar{\mathbf{A}}_0^c, \bar{\mathbf{M}}_{1:T}^c, \bar{\mathbf{F}}_{\frac{1}{2}:T-\frac{1}{2}}^c, \tilde{\mathbf{M}}_T^u) \cdot P(\tilde{\mathbf{M}}_T^u) d\bar{\mathbf{M}}_0^u d\mathbf{F}_{\frac{1}{2}:T-\frac{1}{2}}^u d\tilde{\mathbf{M}}_{1:T}^u \\
&= \int p_{1:T,0:T-1}(\mathbf{M}_{0:T-1}^u, \mathbf{F}_{\frac{1}{2},T-\frac{1}{2}}^u | \bar{\mathbf{L}}_0^c, \bar{\mathbf{A}}_0^c, \bar{\mathbf{M}}_{1:T}^c, \bar{\mathbf{F}}_{\frac{1}{2}:T-\frac{1}{2}}^c, \tilde{\mathbf{M}}_T^u) \cdot P(\tilde{\mathbf{M}}_T^u) d\tilde{\mathbf{M}}_T^u d\bar{\mathbf{M}}_0^u d\mathbf{M}_{1:T-1}^u d\mathbf{F}_{\frac{1}{2}:T-\frac{1}{2}}^u \\
&= \int p_{1:T,0:T-1}(\tilde{\mathbf{M}}_0^u | \bar{\mathbf{L}}_0^c, \bar{\mathbf{A}}_0^c, \bar{\mathbf{M}}_{1:T}^c, \bar{\mathbf{F}}_{\frac{1}{2}:T-\frac{1}{2}}^c, \tilde{\mathbf{M}}_T^u) \cdot P(\tilde{\mathbf{M}}_T^u) d\tilde{\mathbf{M}}_T^u \\
&= p_{1:T,0}(\tilde{\mathbf{M}}_0^u | \bar{\mathbf{L}}_0^c, \bar{\mathbf{A}}_0^c, \bar{\mathbf{M}}_{1:T}^c, \bar{\mathbf{F}}_{\frac{1}{2}:T-\frac{1}{2}}^c)
\end{aligned}$$

where the second equality is from the independence of \mathbf{M}_T^u with respect to $\mathbf{M}_{0:\frac{1}{2}:T}^c$. Then, the Markov structure gives the third equality, and marginal integration gives the last two equalities. By taking average over $\mathbf{M}_{\frac{1}{2}:\frac{1}{2}:T}^c$ for a given constrained structure \mathbf{M}_0^c ,

$$\begin{aligned}
P(\mathbf{M}_0 | \mathbf{M}_0^c) &= \int p_{1:T,0}(\tilde{\mathbf{M}}_0^u | \bar{\mathbf{L}}_0^c, \bar{\mathbf{A}}_0^c, \bar{\mathbf{M}}_{1:T}^c, \bar{\mathbf{F}}_{\frac{1}{2}:T-\frac{1}{2}}^c) \cdot q_{0,\frac{1}{2},\frac{1}{2},T}(\mathbf{M}_{\frac{1}{2}:\frac{1}{2}:T}^c | \mathbf{M}_0^c) d\mathbf{M}_{\frac{1}{2}:\frac{1}{2}:T}^c \\
&= \int p_{1:T,0}(\tilde{\mathbf{M}}_0^u | \bar{\mathbf{L}}_0^c, \bar{\mathbf{A}}_0^c, \bar{\mathbf{M}}_{1:T}^c, \bar{\mathbf{F}}_{\frac{1}{2}:T-\frac{1}{2}}^c) \cdot q_{0,\frac{1}{2},\frac{1}{2},T}(\bar{\mathbf{L}}_0^c, \bar{\mathbf{A}}_0^c, \bar{\mathbf{M}}_{1:T}^c, \bar{\mathbf{F}}_{\frac{1}{2}:T-\frac{1}{2}}^c | \tilde{\mathbf{M}}_0^c) d\bar{\mathbf{L}}_0^c d\bar{\mathbf{A}}_0^c d\bar{\mathbf{M}}_{1:T}^c d\bar{\mathbf{F}}_{\frac{1}{2}:T-\frac{1}{2}}^c \\
&\approx q_{0,0}(\tilde{\mathbf{M}}_0^u | \tilde{\mathbf{M}}_0^c),
\end{aligned}$$

i.e., the conclusion we have before also hold for the DiffCSP case where there is Predictor-Corrector mechanism in the denoising generative model.

V Training of the generative model

To train DiffCSP architecture, we used the MP-20^{6,7} dataset of 45231 materials from the Materials Project database. MP-20 covers 89 elements, as Figure S11 shows the element distribution for each of the train, validation, and test datasets. MP-20 includes most experimentally known materials with up to 20 atoms per unit cell. All materials are selected from the stable ones after DFT relaxation. MP-20 includes materials with energy above the hull (E_{hull}) smaller than 0.08 eV/atom and formation energy smaller than 2 eV/atom.

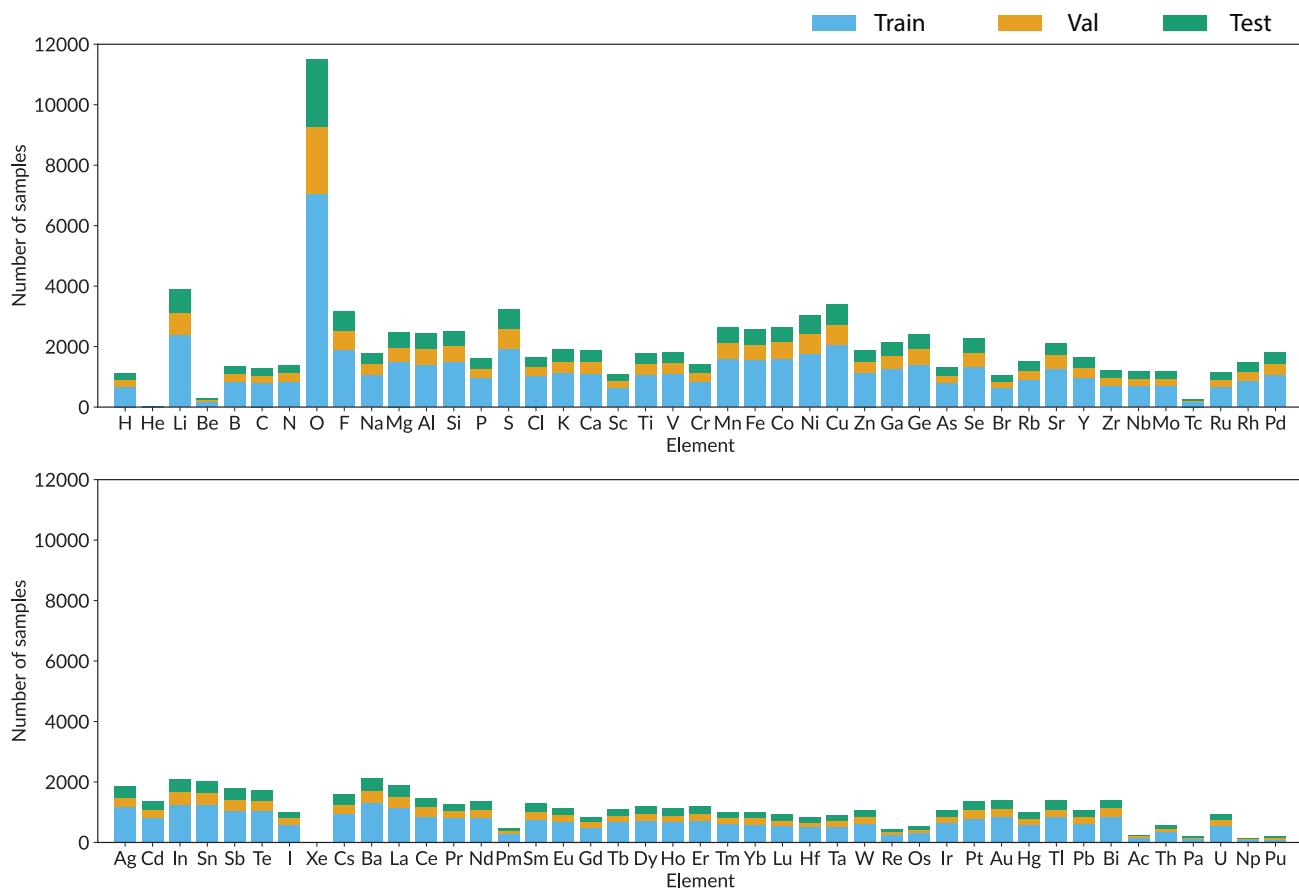


Figure S11. Training and testing data by elements in the MP-20 dataset. The number of appearances by each chemical element in the training (blue), validation (orange), and testing (green) datasets.

VI Stability pre-screening procedures of generated materials

It is crucial to investigate whether the generated materials are stable to determine the candidate materials for density functional theory (DFT) calculations and for further practical application. In our work, we present a four-staged stability screening that is quick and efficiently removes unrealistic samples. The first two filters are straightforward: charge neutrality and the ratio of unit cell space occupied by atoms. Each crystal needs to be neutral about its electrical charge. We used the SMACT⁸ library to search if each material could meet this requirement. Additionally, we considered the ratio of the space occupied by the atoms per the volume of the unit cell. As the violin plots in Fig. S12 show, the space occupation ratio R_{occ} ranges in a similar manner over different N values in the MP-20 dataset. Among the materials generated by SCIGEN, some exhibit excessively high R_{occ} values, indicating that too many or large atoms are confined within a narrow space of the unit cells. We set $R_0 = 1.7$ as the threshold, which is slightly higher than the maximum R_{occ} for each N in Figure S12, and discarded the materials with higher R values than R_0 .

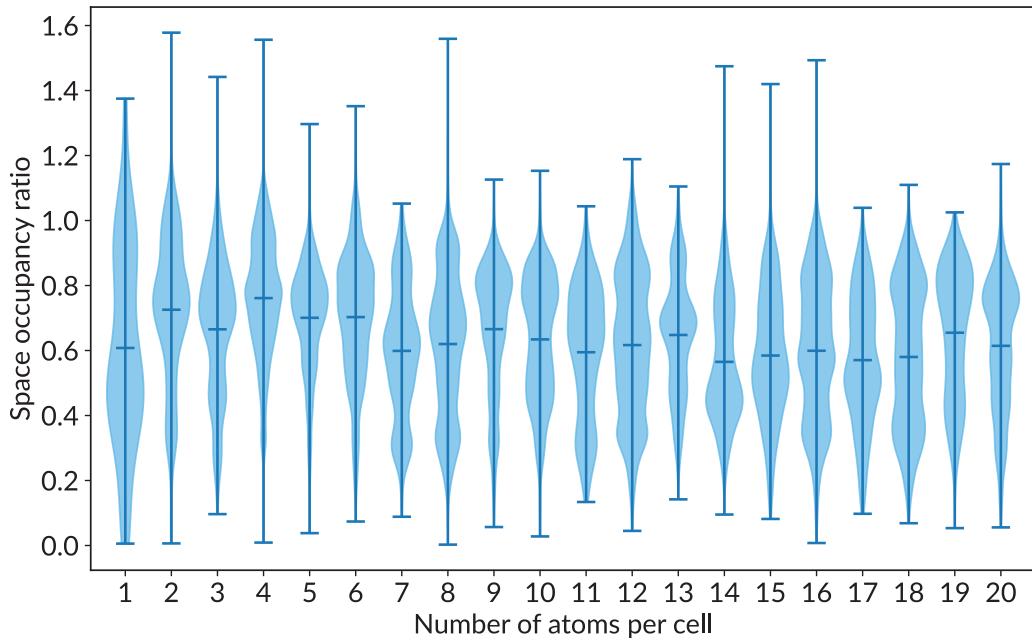


Figure S12. Space occupancy distribution of MP-20 dataset. We surveyed the space occupancy ratio of the 45229 materials in the MP-20 dataset. The highest value is 1.578.

Next, we built classification models based on Graph Neural Networks (GNN) that take crystal structures as input. Evaluation of the crystal structure stability needs to take the atom types and their geometric relations into account, and GNNs are capable of dealing with these together. To learn the stable phases from the existing material database, we trained two GNN models, Ψ_1 and Ψ_2 , as simple and fast tools. Ψ_1 was trained to classify whether the given materials present energy above the convex hull (E_{hull}) higher or lower than 0.1 eV. We set E_{hull} lower than 0.1 eV as the stable samples. We accessed the materials with the E_{hull} values from the Matbench Discovery⁹. Ψ_2 was designed to evaluate if the input materials are pristine and distinctive from diffused structures. This model was trained to classify pristine materials in the MP-20^{6,7} dataset and those diffused by Gaussian noise with 5% deviation. We implemented GNN models Ψ_1 and Ψ_2 using E3NN library^{10,11}. Figure S13 shows the confusion matrices for the two GNN models, which confirm their capabilities for stability classification.

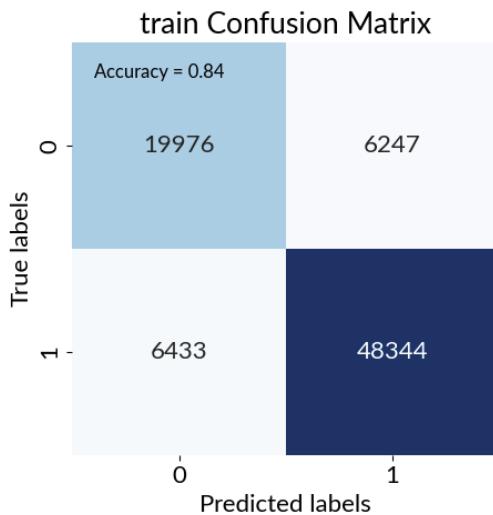
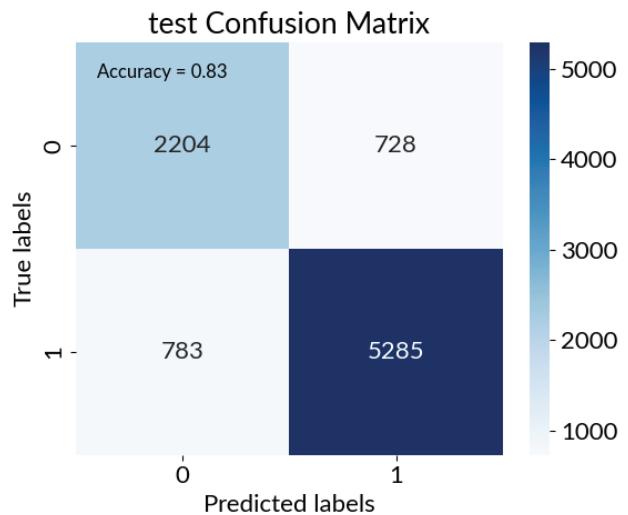
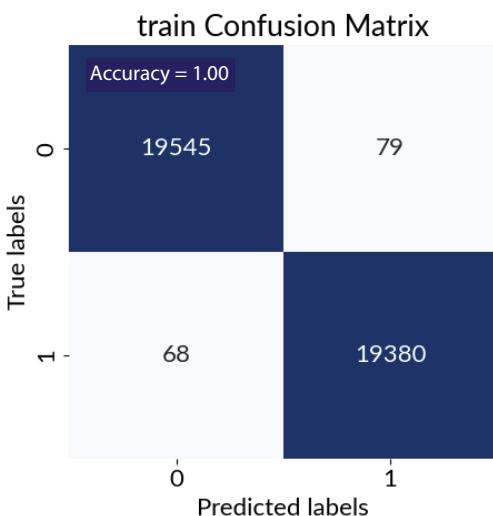
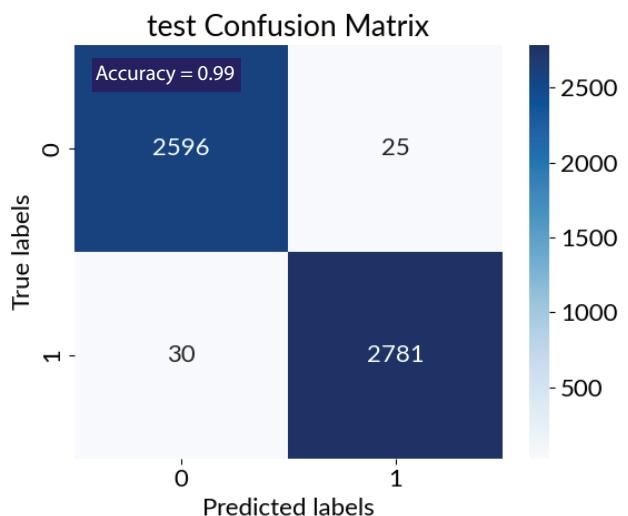
a**b****c****d**

Figure S13. Confusion matrix of GNN-based stability classifier. The class labels '1' and '0' indicate stable and unstable, respectively. **a.** Training data of E_{hull} classification (Ψ_1). **b.** Test data of E_{hull} classification (Ψ_1). **c.** Training data of diffused structure classification (Ψ_2). **d.** Test data of diffused structure classification (Ψ_2).

Using the criteria described above, we pre-screened the generated materials. Table S2 provides the ratio of survived materials relative to the total generated material structures after each filter. We named the pre-screening procedures of charge neutrality, space occupation ratio, Ψ_1 , and Ψ_2 as Filters 1 through 4, respectively. Approximately 6 to 8 percent of the generated materials passed the filters when we imposed the geometry of Triangular, Honeycomb, and Kagome lattice layers. Compared to DiffCSP, the survival ratio is lower by an order. This difference arises from the constraints of specific geometry within the crystal structures, which can lead to higher failure rates compared to the vanilla model without rigorous imposition of structures. However, we were able to generate new materials with AL geometries, which are rare and can potentially expand the boundaries of the existing material database.

Table S2. Pre-screening evaluation

AL	Triangular	Honeycomb	Kagome	DiffCSP
Filter 1	92.14	83.90	66.44	81.43
Filter 2	86.13	83.15	65.99	81.43
Filter 3	40.89	24.24	19.91	64.38
Filter 4	6.13	7.33	8.35	62.54

For the three AL types (Triangular, Honeycomb, Kagome), we tracked the ratio of materials passing the pre-screening filters at each timestamp $t \in [T, 0]$. More materials could pass the filters as the structures are denoised, or in other words, as t gets smaller. This trend indicates that the denoising method optimizes the components of $\mathbf{M}_t = (\mathbf{F}_t, \mathbf{L}_t, \mathbf{A}_t)$ into suitable values. Especially with high enough t close to $T=1000$, the elements of the lattice matrix \mathbf{L}_t can be approximated to follow a normal distribution. Consequently, the volume of the unit cell is significantly smaller than that of actual crystals. Therefore, almost no samples pass the criteria of space occupation ratio (Filter 2), resulting in a narrow area below the green line with a large t region.

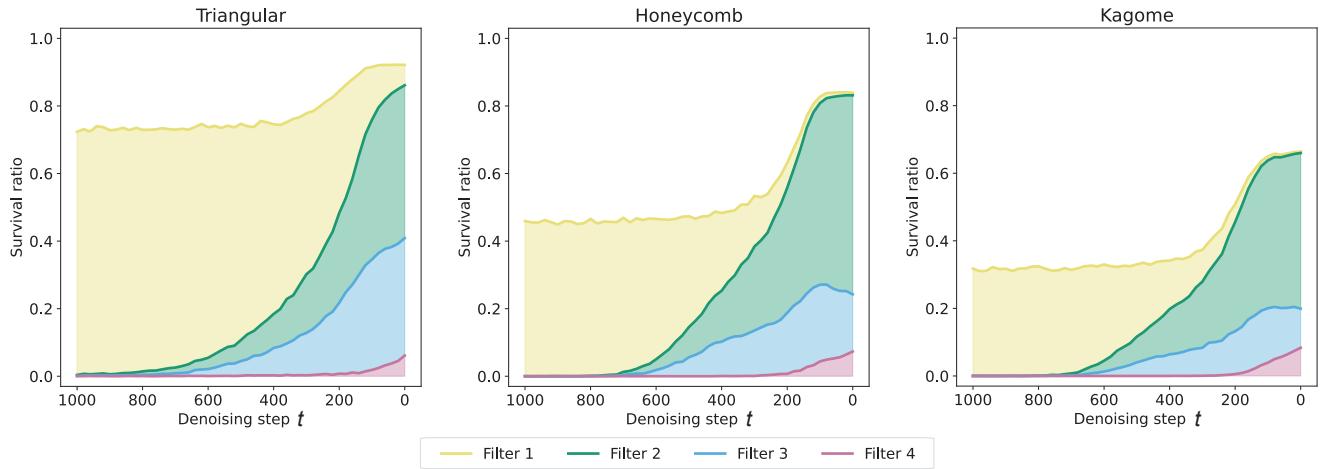


Figure S14. The survival ratio of materials under pre-screening through denoising process. Filter 1, Filter 2, Filter 3, and Filter 4 represent the criteria of charge neutrality, density, energy above the convex hull, and diffusiveness, respectively.

VII Generated materials with Archimedean Lattice constraints

We present the database of the generated materials based on Archimedean lattice (AL) structures. This involves mass generation of materials, pre-screening, density functional theory (DFT) calculations, and evaluation of the stability and novelty of the generated materials.

To create the material database, we first generated materials with AL constraints using our SCIGEN framework. For each sample, we sampled the atom types as the AL vertices \mathcal{A}^c from the uniform distribution of the 10 magnetic atoms (Mn, Fe, Co, Ni, Ru, Nd, Gd, Tb, Dy, and Yb). We then sampled the distances d^c between the nearest neighbor vertices from the KDE in Fig. S2. We sampled the number of atoms per unit cell N from the generated profile in Fig. S7. To regulate the complexity of generated materials, we specified N_{\max} , the maximum value of N , as $\min(4N^c, 20)$ for each AL. After all, the whole dataset contains 7.87 million materials.

We pre-screened the initially generated materials to ensure a manageable and diverse dataset for further analysis by DFT. We first applied the four-layered pre-screening filters, which we mentioned in Supplementary Information 5, to narrow down the outputs to 790 thousand. Subsequently, we employed DFT for the structure relaxation of these materials. The DFT calculations were performed on 26,000 materials down-sampled from the 790 thousand, resulting in 13.8 thousand stable phases. Stability was evaluated based on three primary metrics derived from the DFT results: maximum interatomic force after relaxation (F_{\max}), average changes in lattice constants (d_{latt}), and average changes in atomic coordinates (d_{xyz}). For a material to be considered stable, we set the upper bound for F_{\max} to 0.01 eV/Å. To evaluate the degree of structural changes through DFT, the thresholds for d_{latt} and d_{xyz} were determined specifically for each class of AL structures. To ensure the novelty of the generated materials, we filtered out duplicates from the dataset. This process involved two main steps: first, identifying structural matches with the MP-20 training dataset. We used StructureMatcher from Pymatgen¹² to evaluate the correspondence of the structures. Second, we removed materials with identical structures within the generated set. When multiple outputs presented the same crystal structures, we retained the one with the lowest d_{xyz} value to ensure the highest precision in atomic positioning.

Table S3 presents the threshold values of d_{latt} and d_{xyz} (Å) and the number of materials that remained after each filtration step. Our analysis revealed that materials with square lattice structures exhibited relatively lower novelty due to the prevalence of similar structures in the dataset, typically consisting of 2 atoms per unit cell with a cubic lattice. Conversely, other AL types demonstrated significantly higher novelty, indicating that our generative method effectively produced materials outside the known distribution. Furthermore, materials that passed all the criteria are presented in Fig. S15-S218. For Lieb-like lattice materials, we present the calculated band structures of each material structure. We cover all of the stable materials ($F_{\max} < 0.01$ eV/Å) in Table S4-S14. Note that the bold IDs in these tables mean the materials meeting the criteria of F_{\max} , d_{latt} and d_{xyz} , which we display the crystal structures in Fig. S15-S218.

Finally, it is noteworthy that generating stable materials with the Great rhombitrihexagonal (*grt*) lattice structures proved to be particularly challenging under the current constraints. As such, further work is required to address these difficulties and is planned for future studies.

Table S3. The threshold values of distortion (d_{latt} and d_{xyz}) and the counts of materials survive after DFT

Archimedean lattice	d_{latt}	d_{xyz}	(1) Stable (F_{\max})	(2) Small distortion ($d_{\text{latt}}, d_{\text{xyz}}$)	(3) Novel structures (wrt MP-20 train)	(4) Remove duplicates
Triangular	1.0	0.5	2584	1692	1544	765
Honeycomb	1.0	0.5	1829	250	245	235
Kagome	1.0	0.5	1489	452	439	392
Square	1.0	0.5	2754	2363	1679	538
Elongated triangular	1.0	0.5	1356	127	127	125
Snub square	1.0	0.5	957	134	132	131
Truncated square	2.0	1.0	553	143	143	143
Small rhombitrihexagonal	2.0	1.0	736	305	305	268
Snub hexagonal	2.0	1.0	668	212	212	191
Truncated hexagonal	3.0	1.5	125	40	40	40
Lieb	1.0	0.5	829	213	205	190

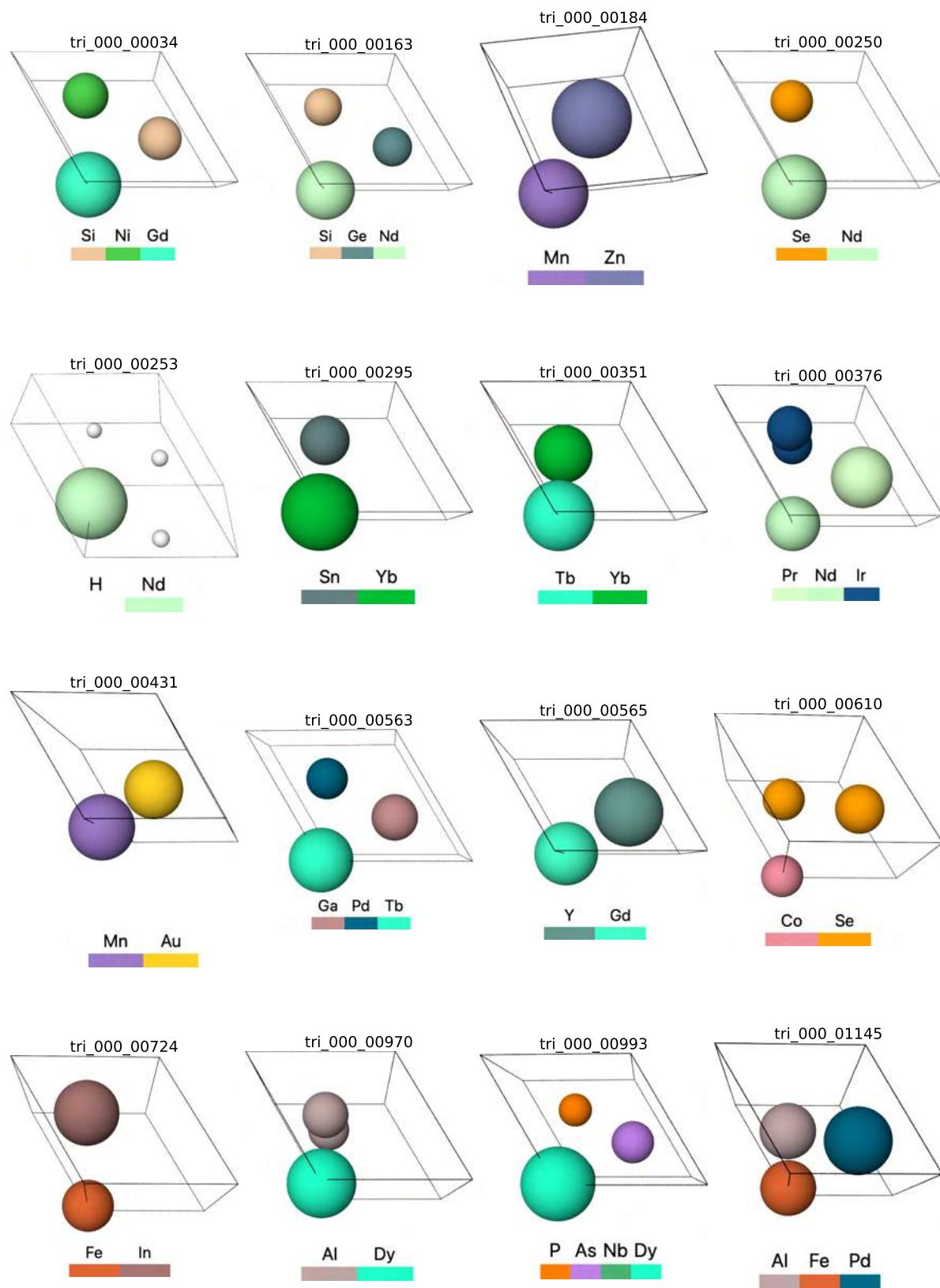


Figure S15. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

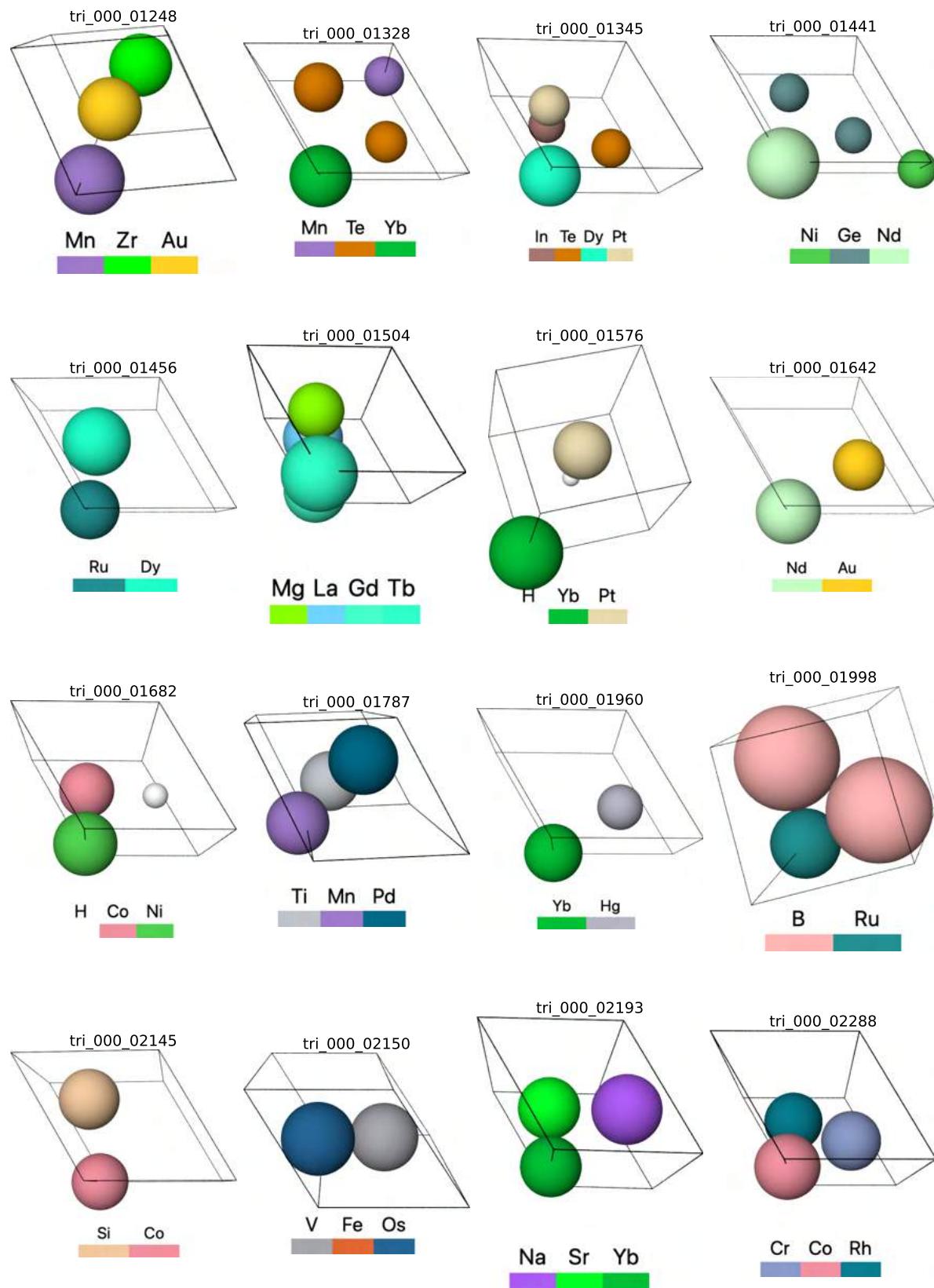


Figure S16. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

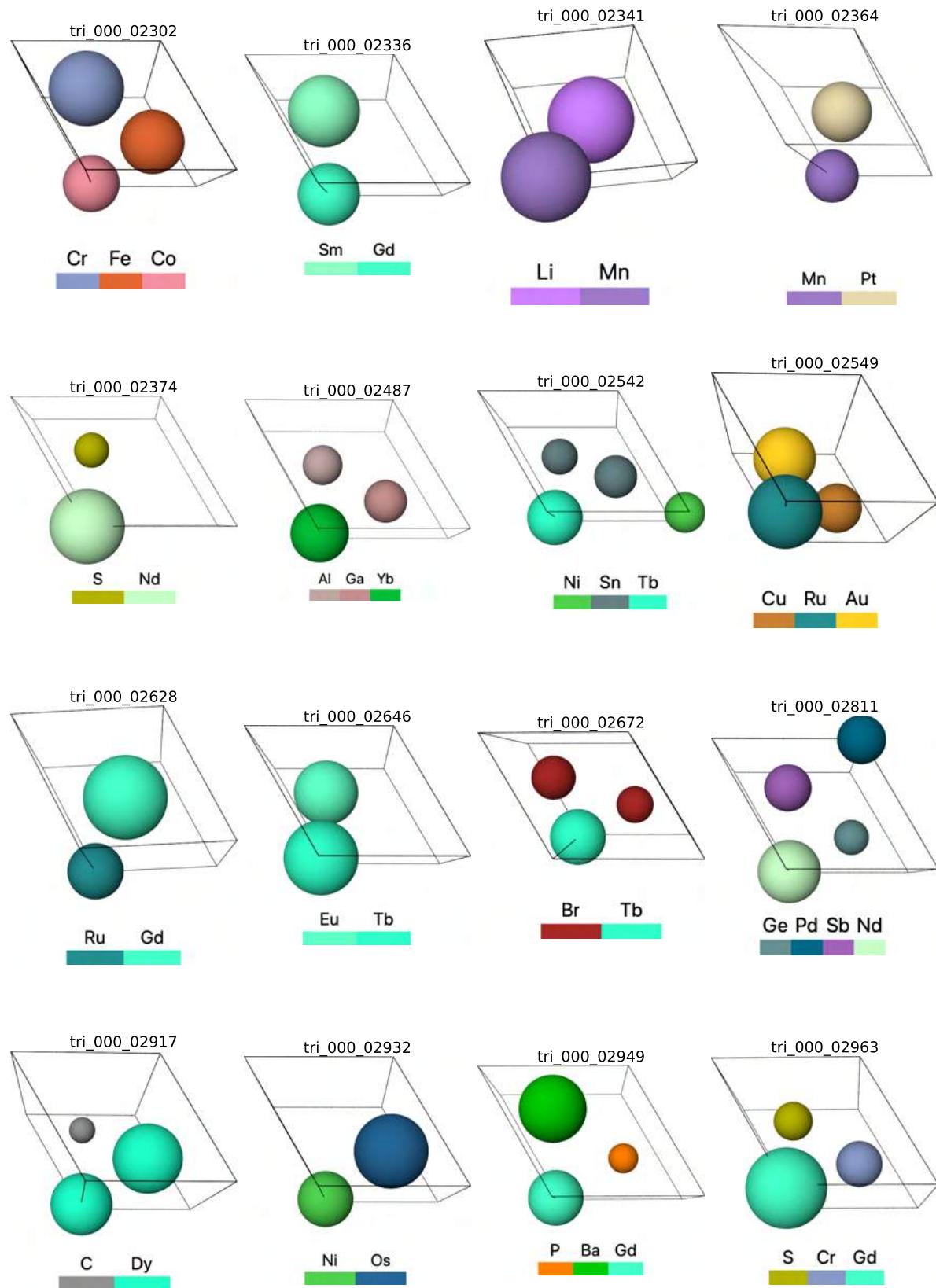


Figure S17. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

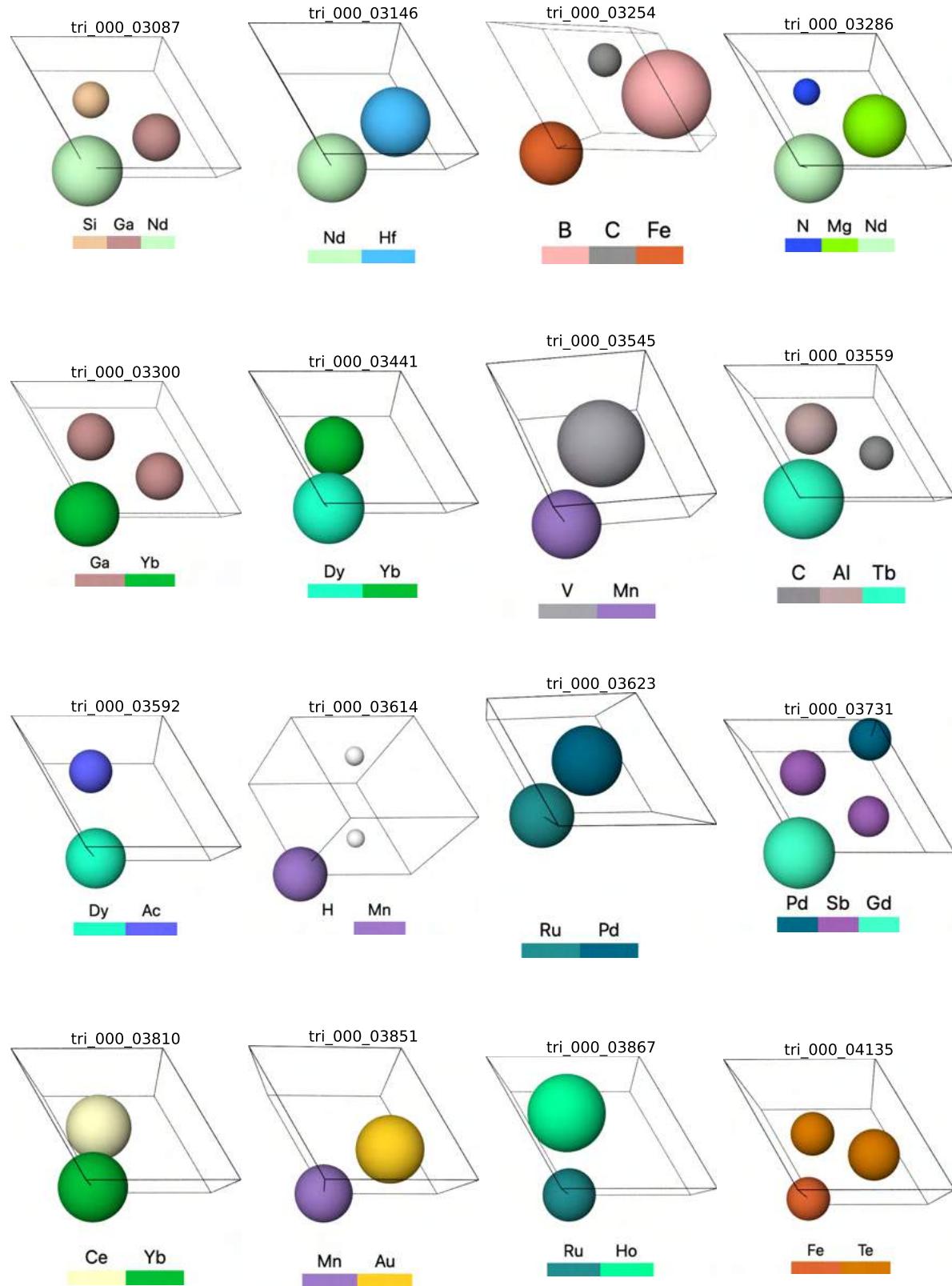


Figure S18. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

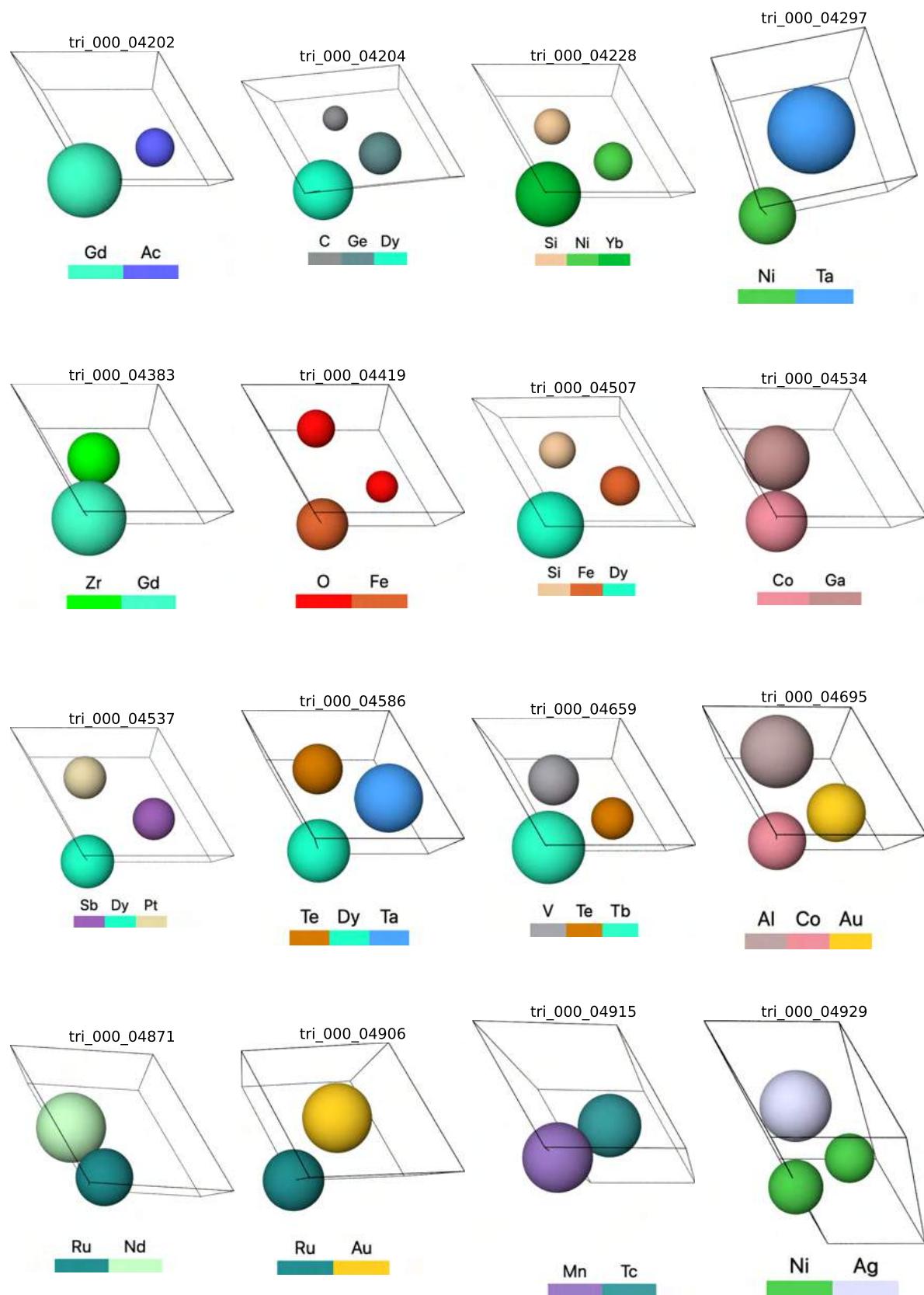


Figure S19. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

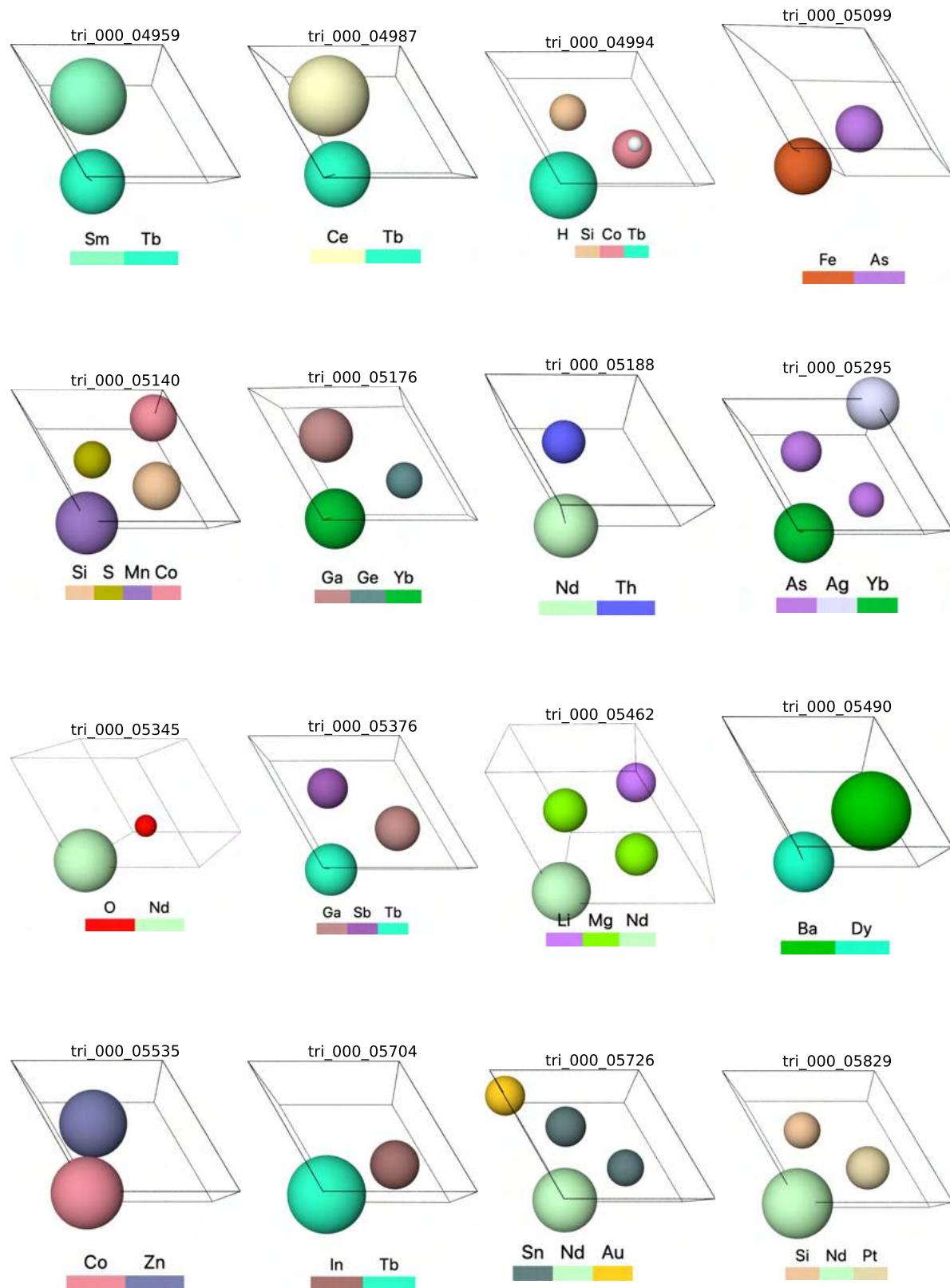


Figure S20. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

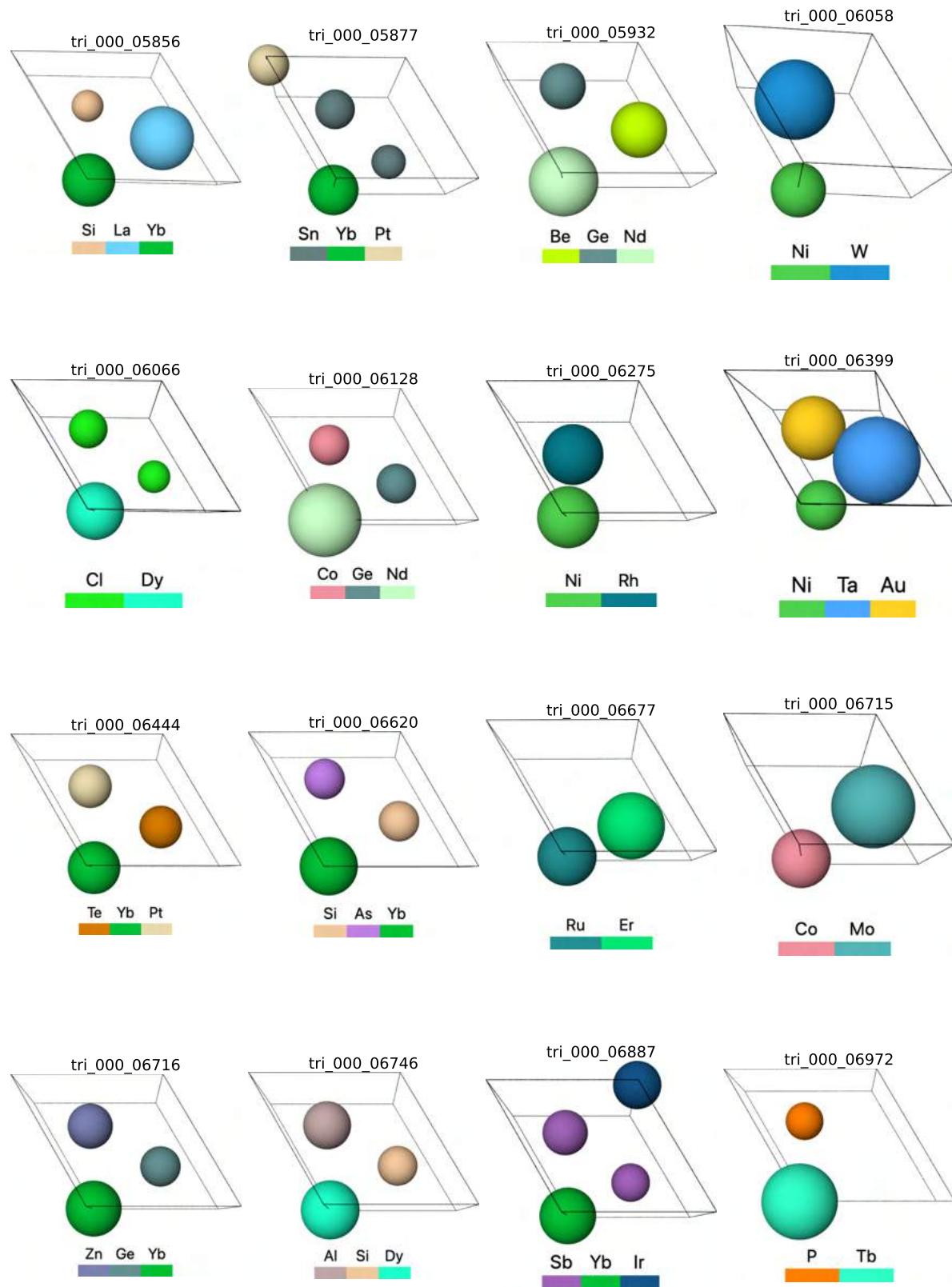


Figure S21. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

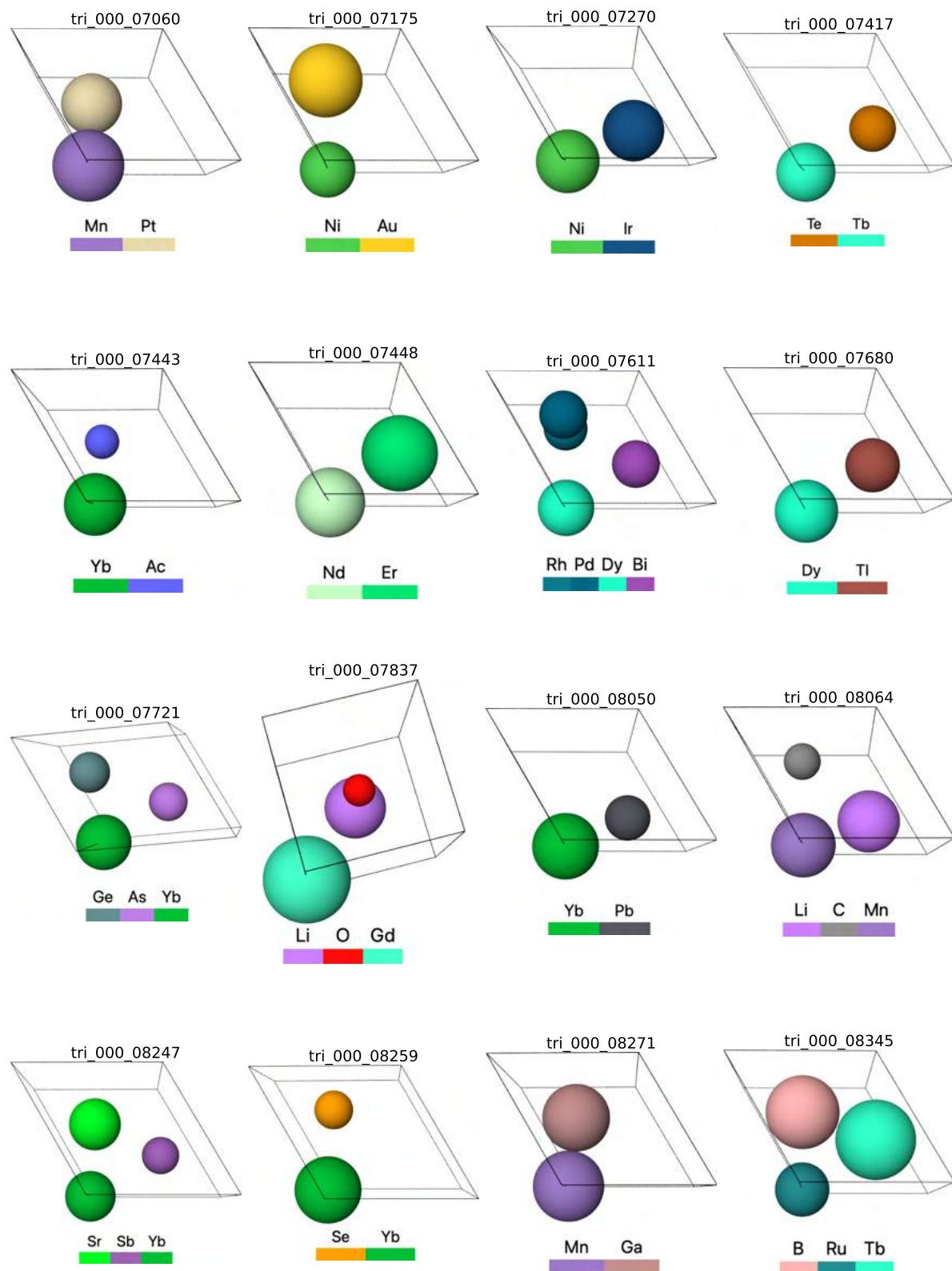


Figure S22. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

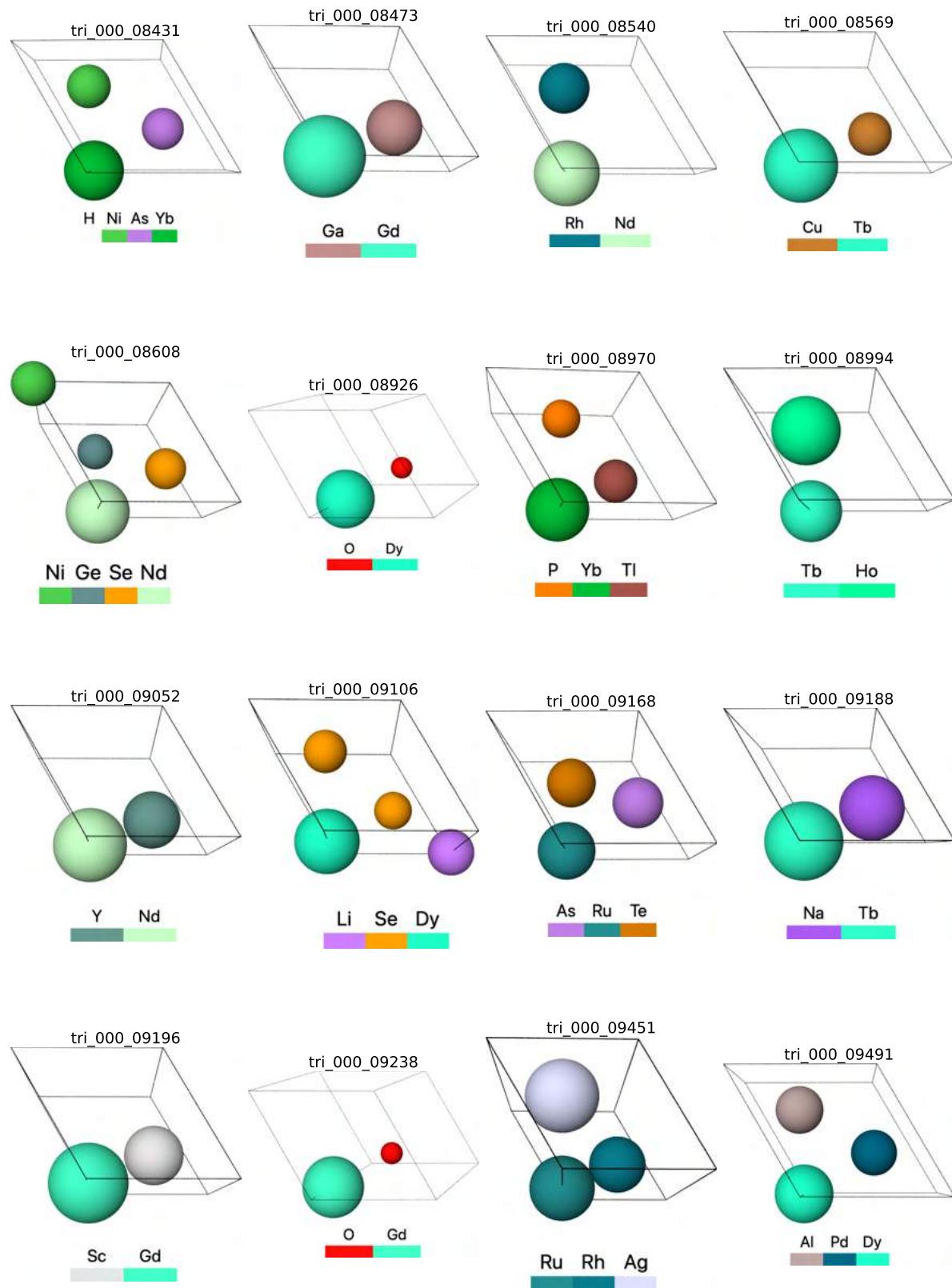


Figure S23. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

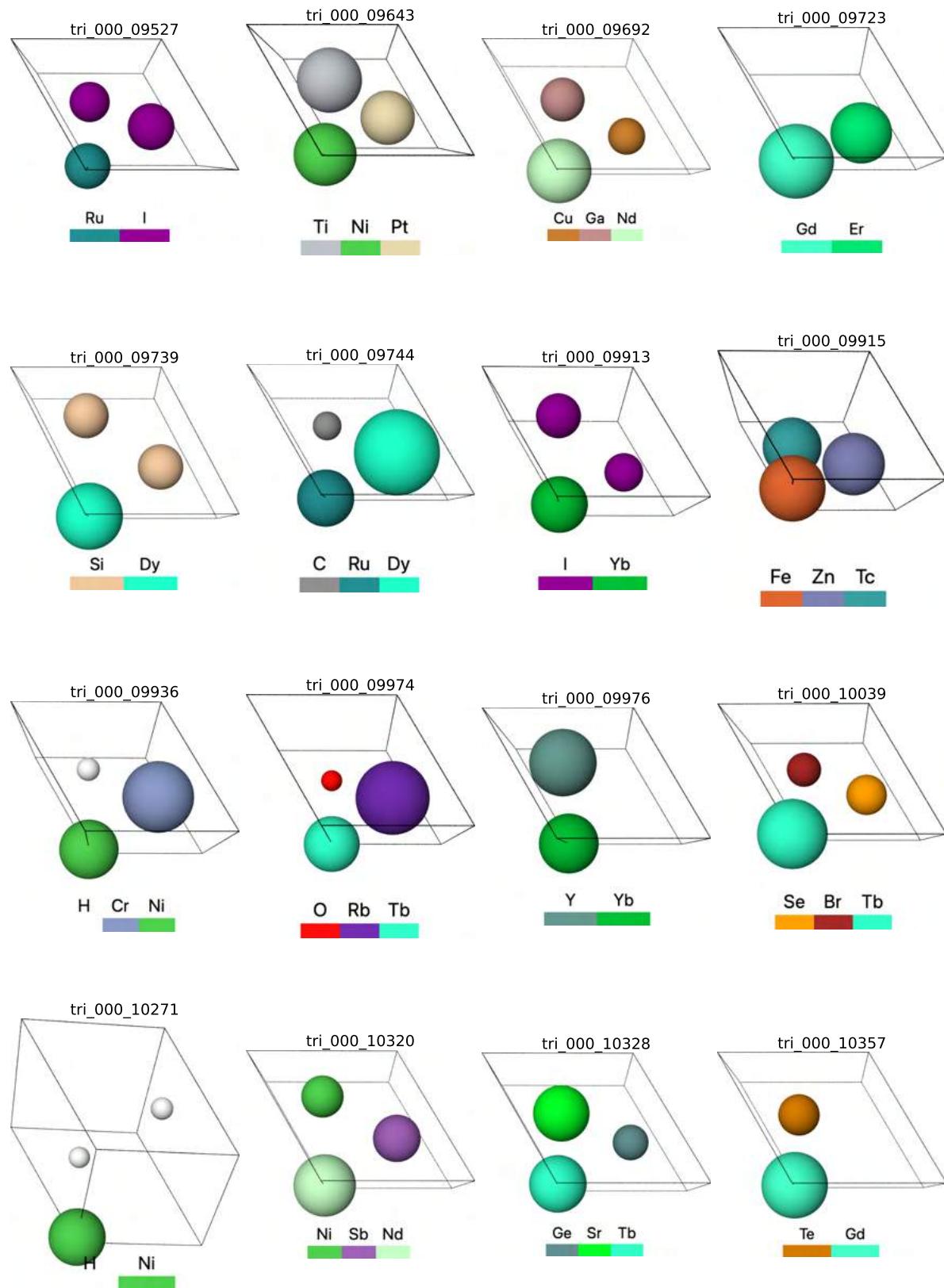


Figure S24. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

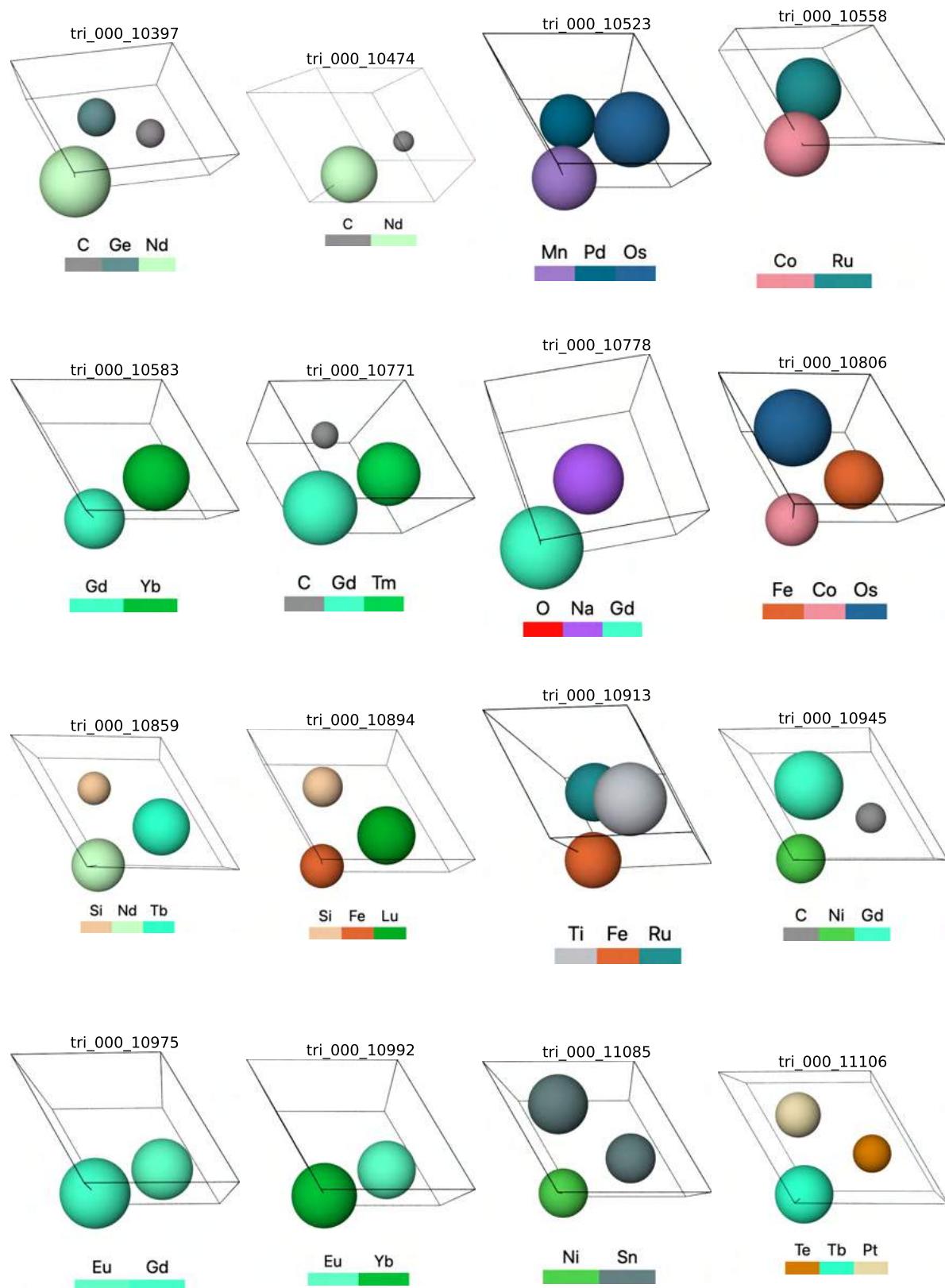


Figure S25. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

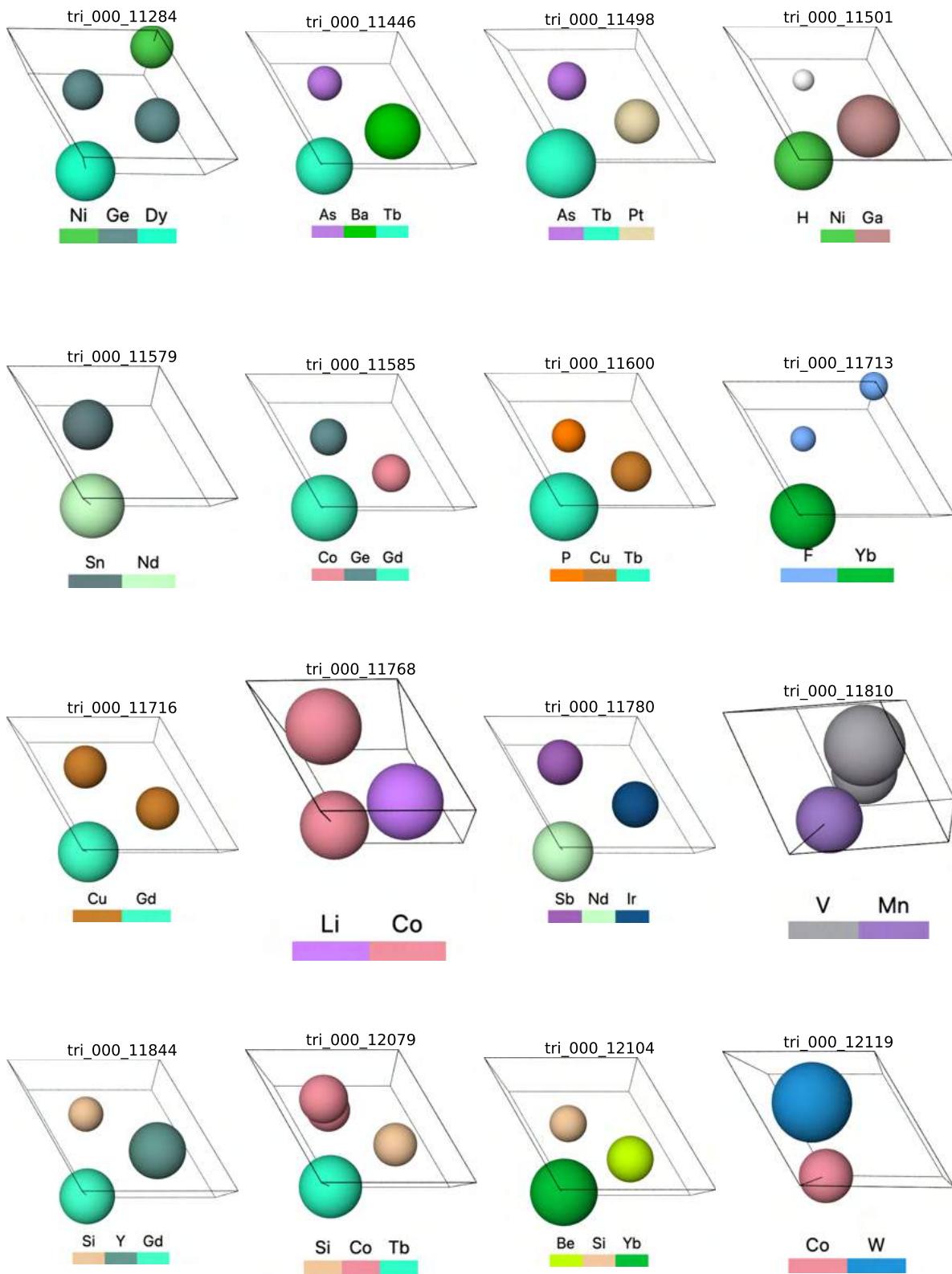


Figure S26. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

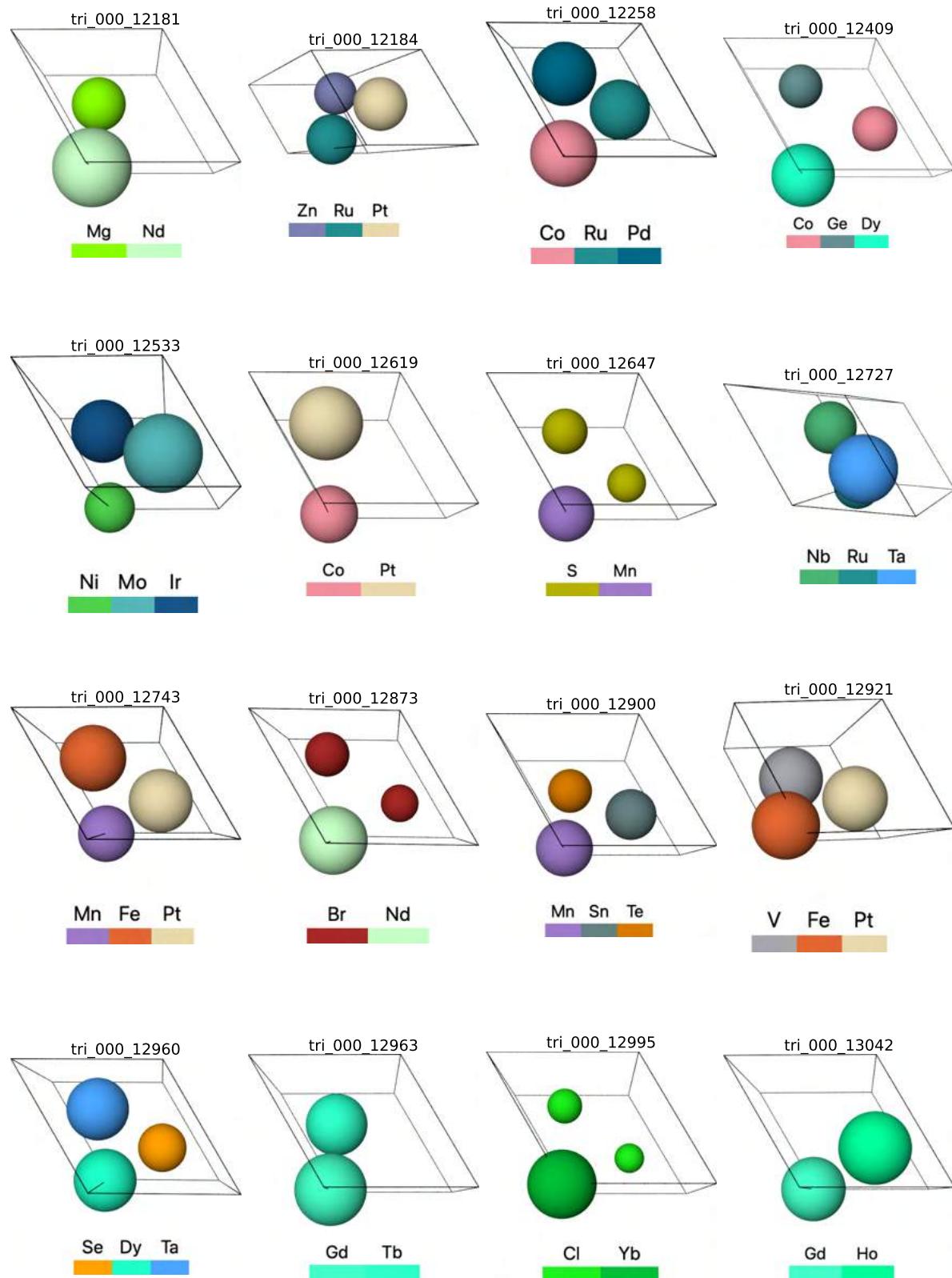


Figure S27. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

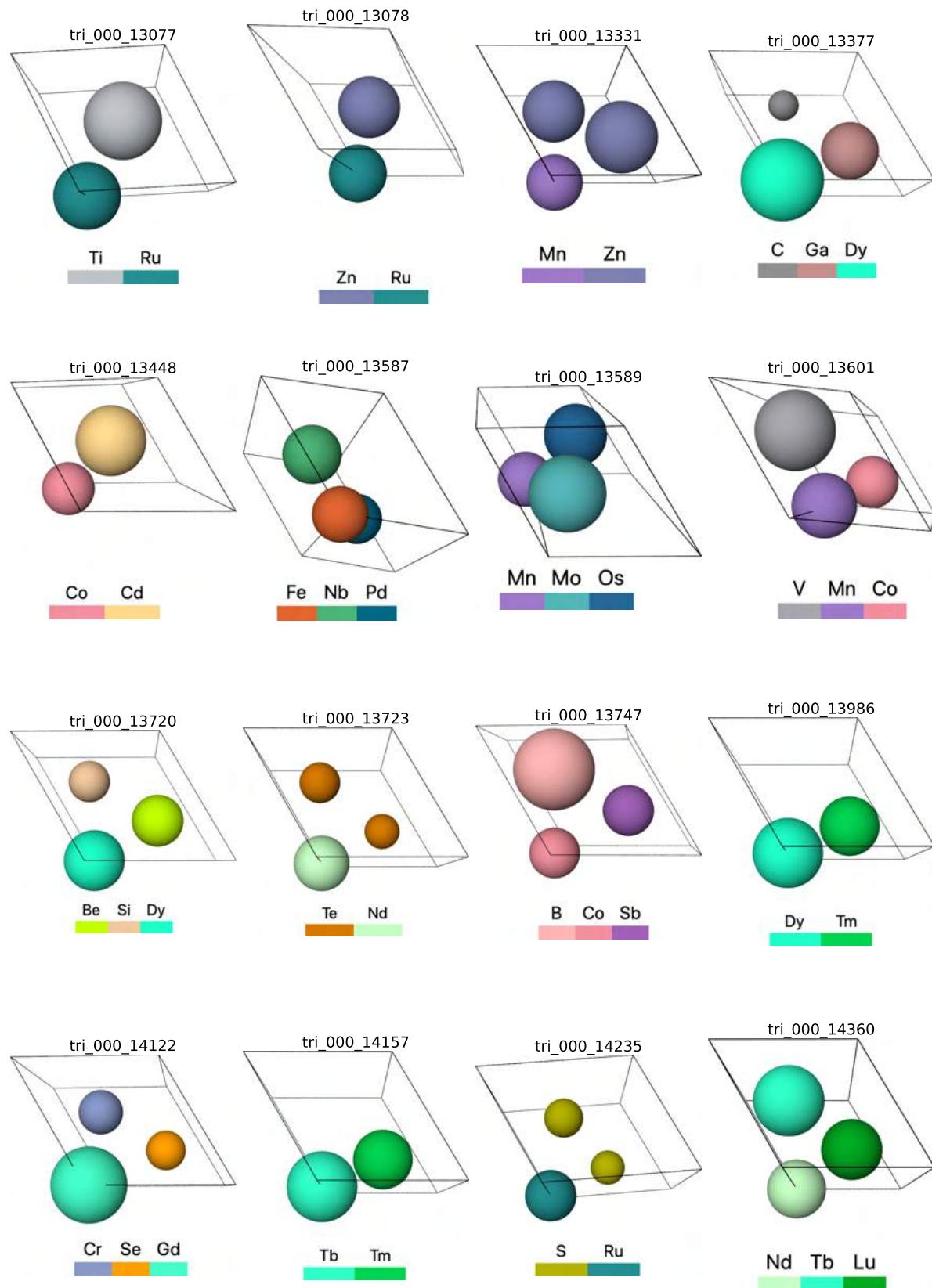


Figure S28. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

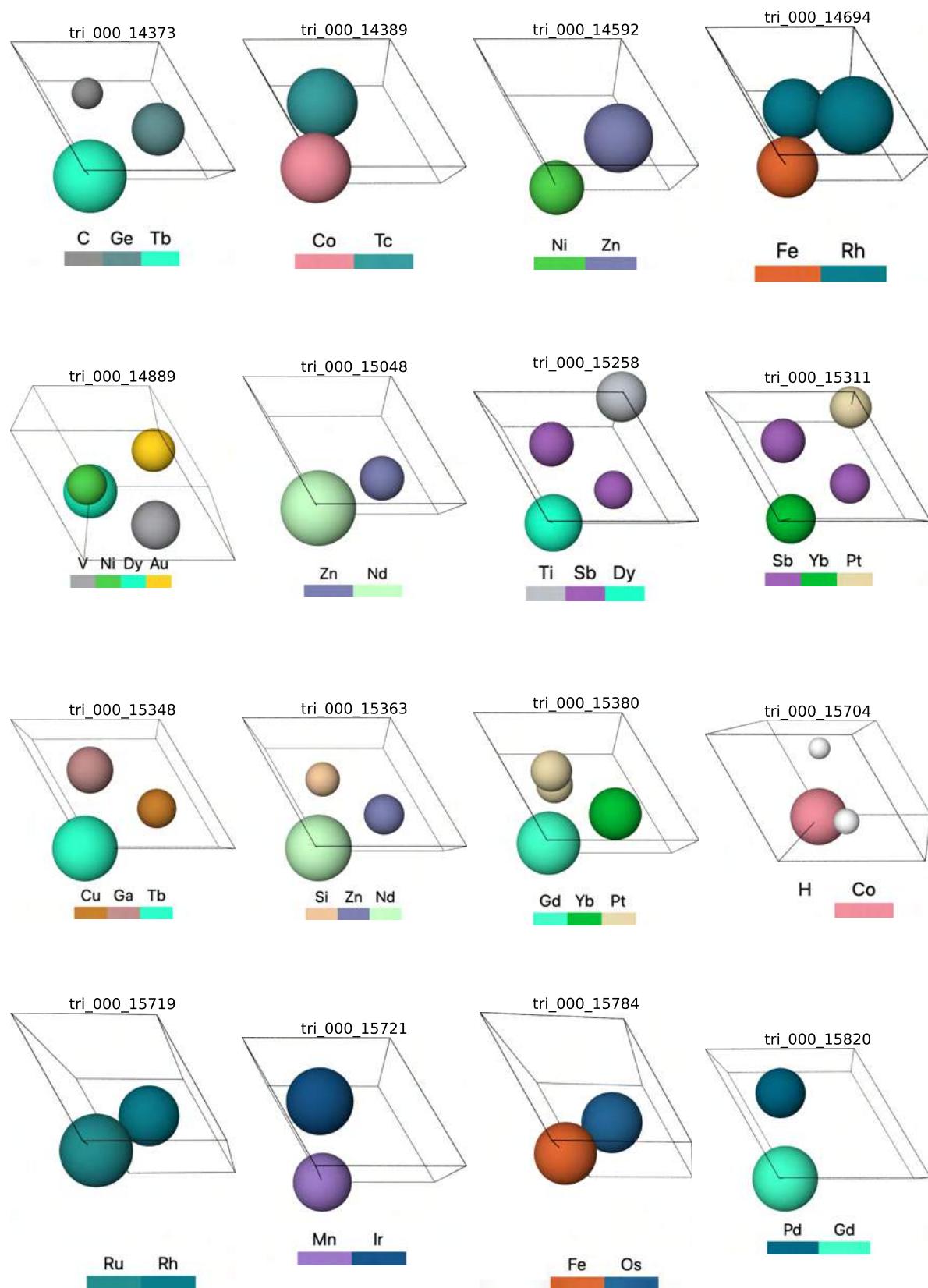


Figure S29. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

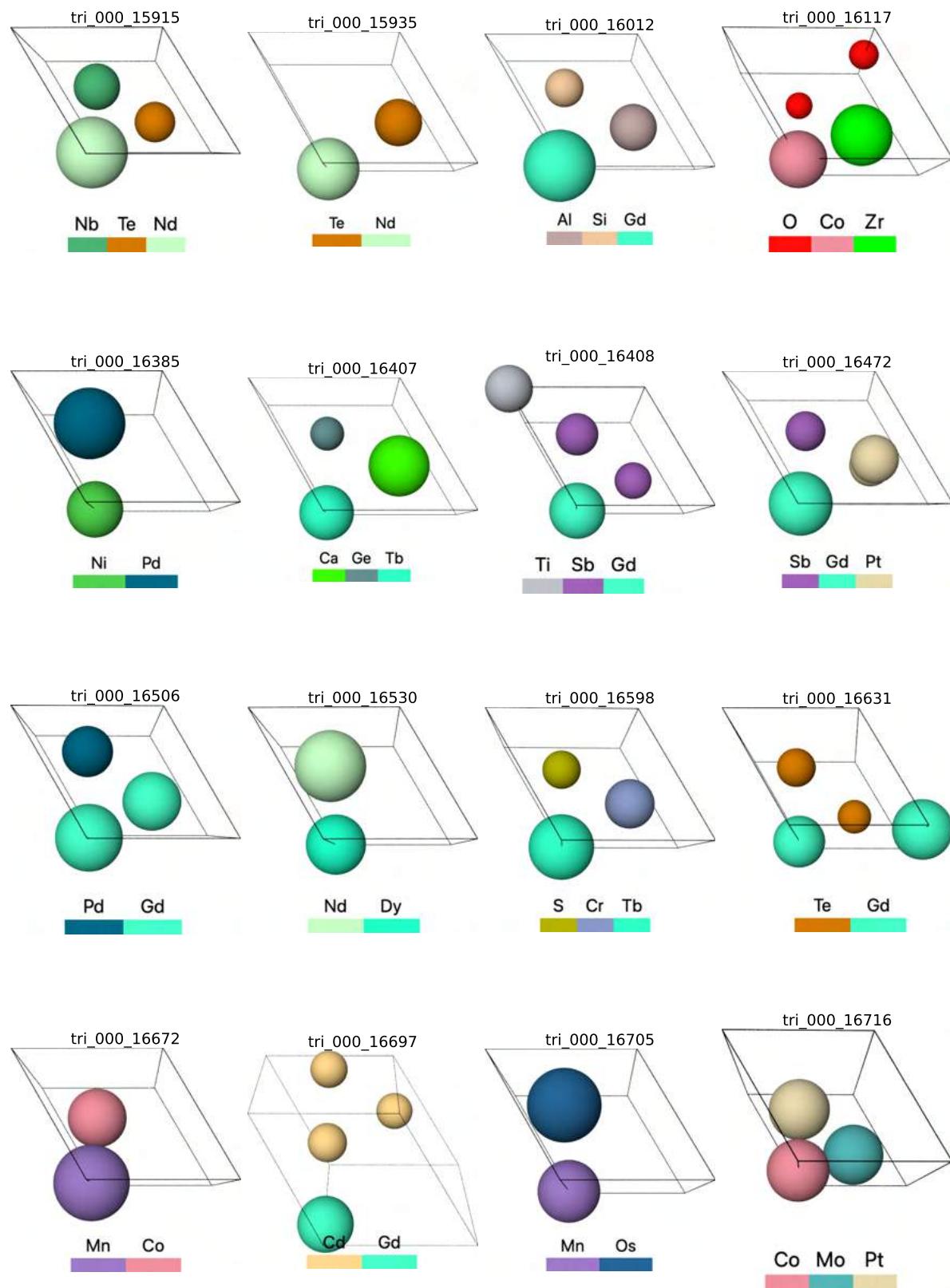


Figure S30. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

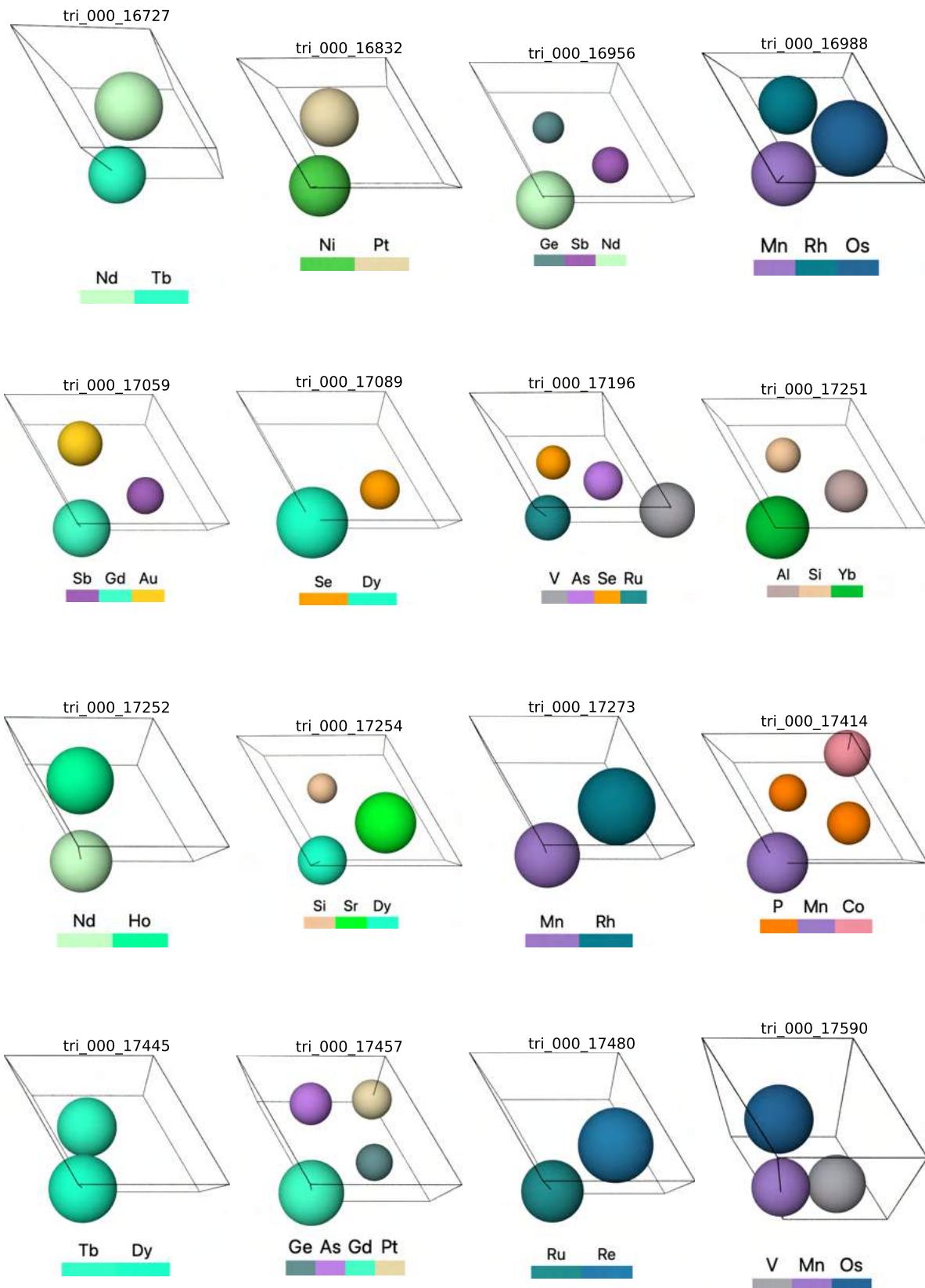


Figure S31. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

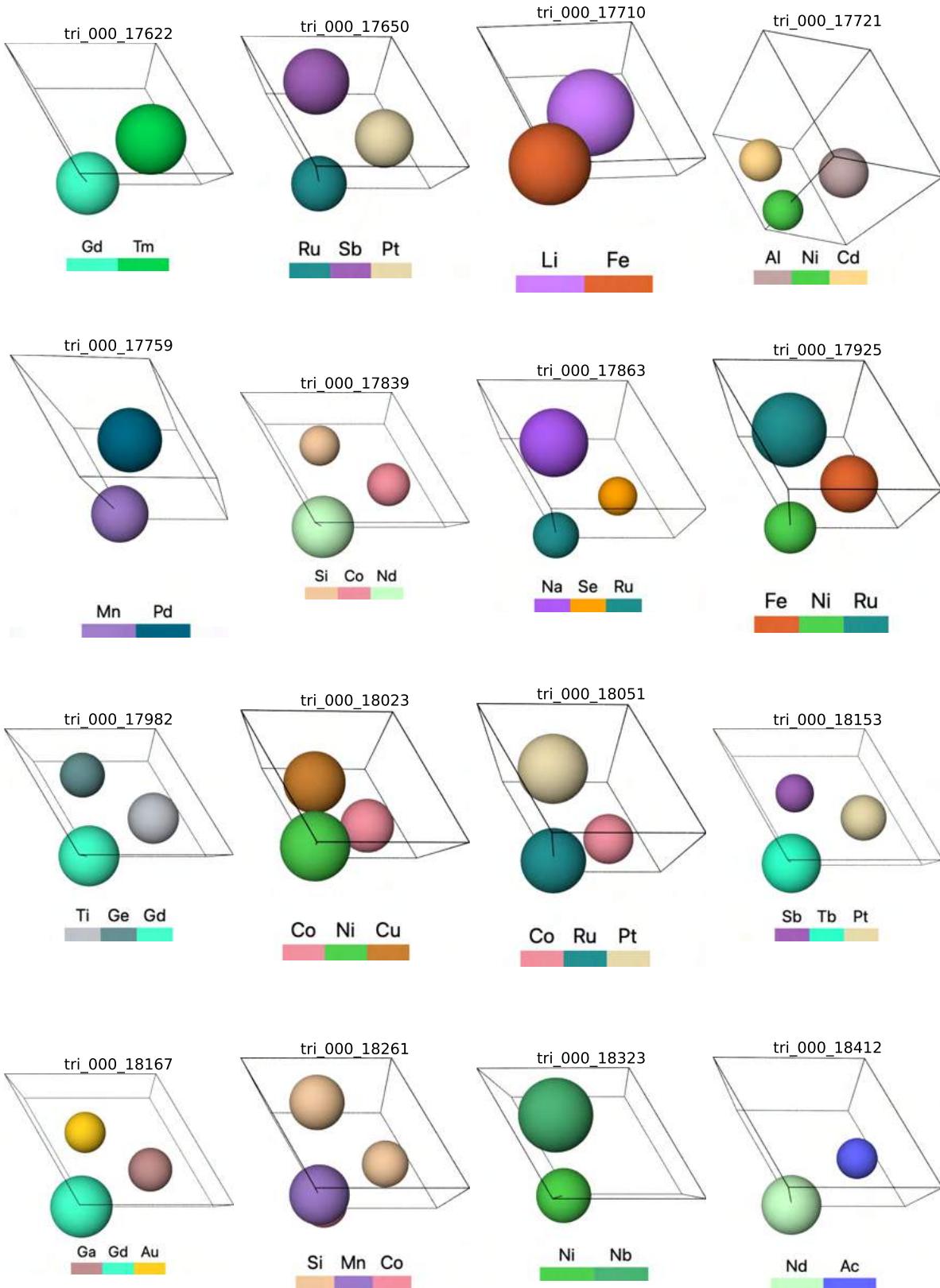


Figure S32. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

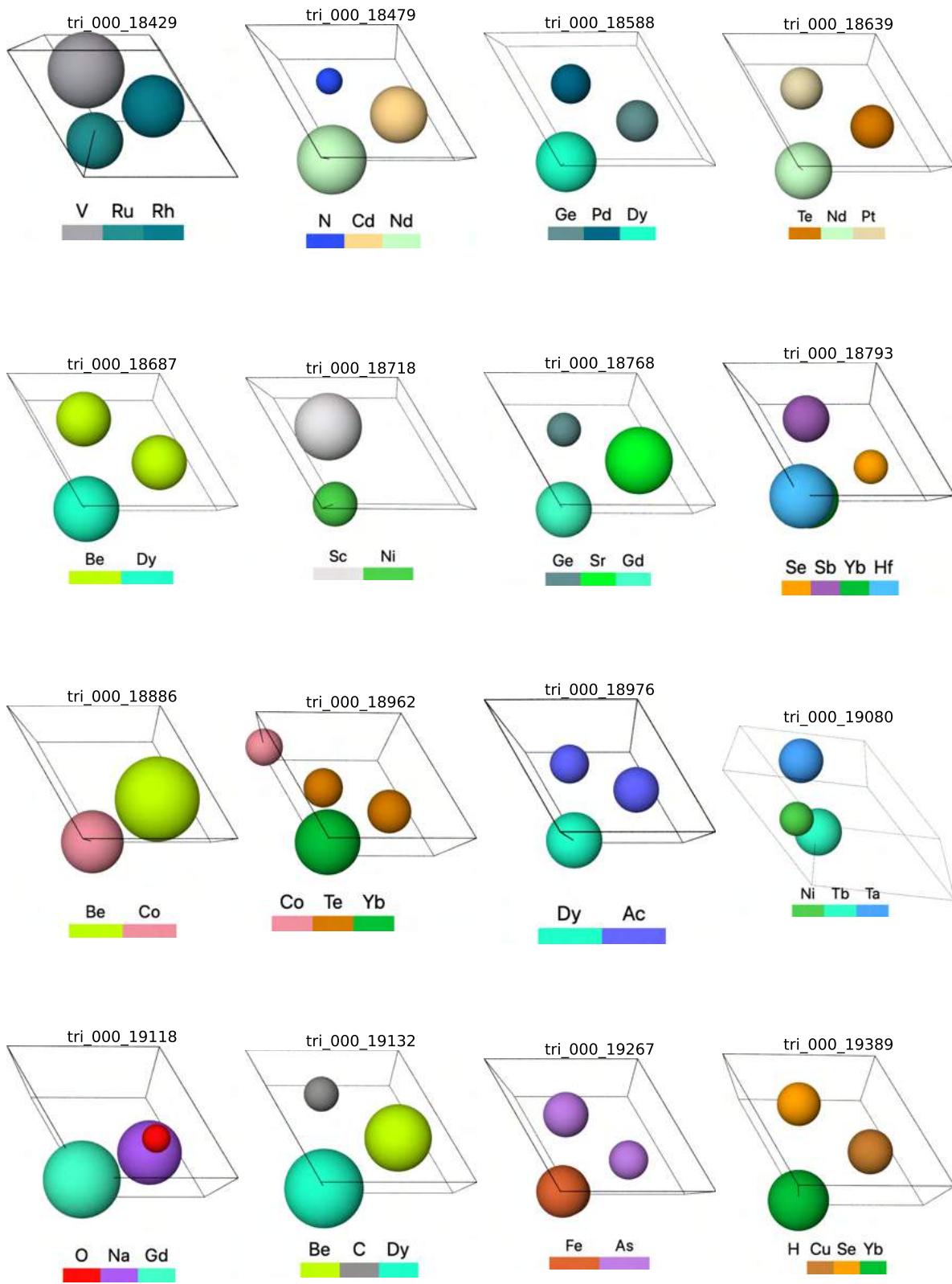


Figure S33. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

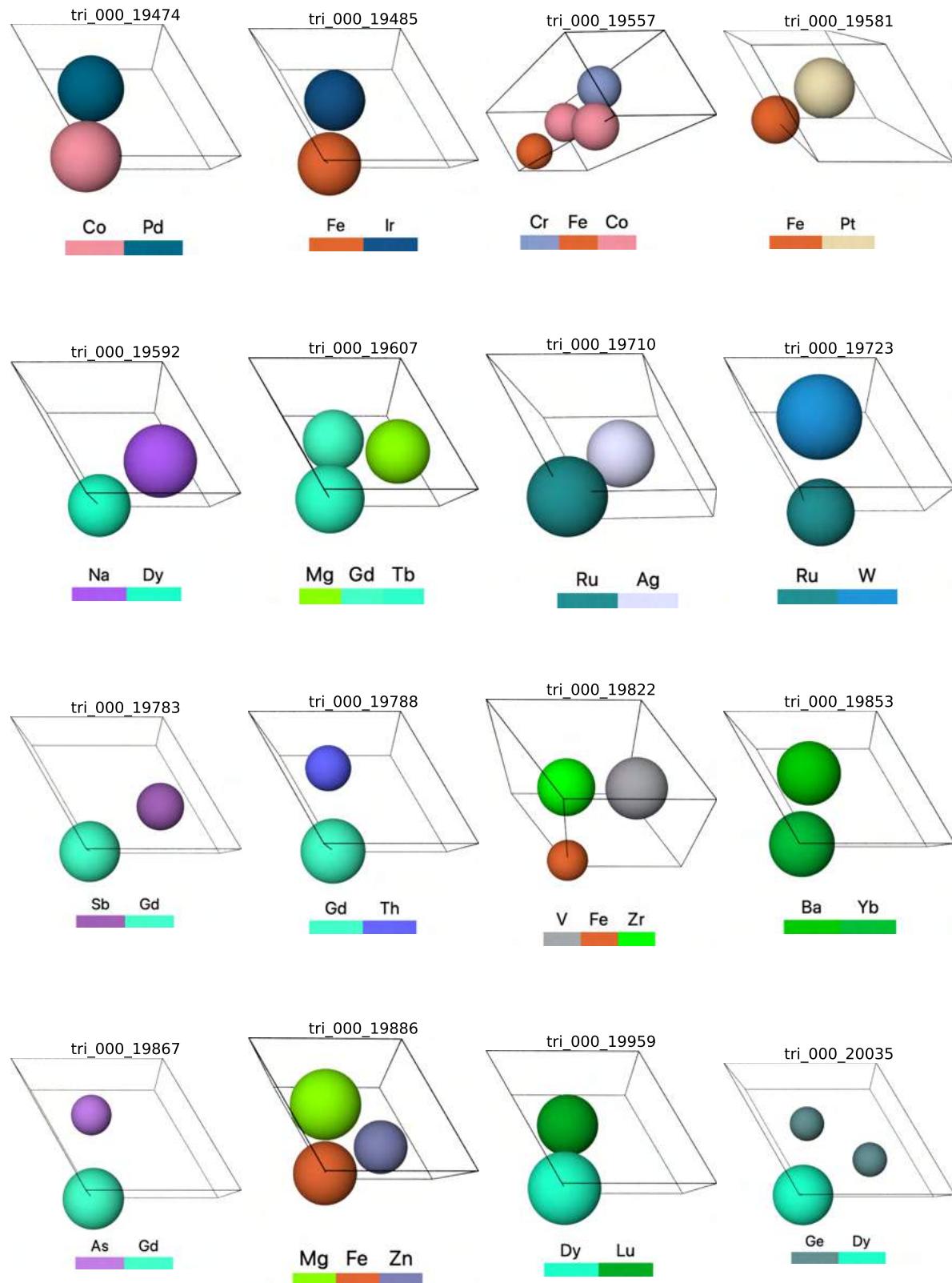


Figure S34. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

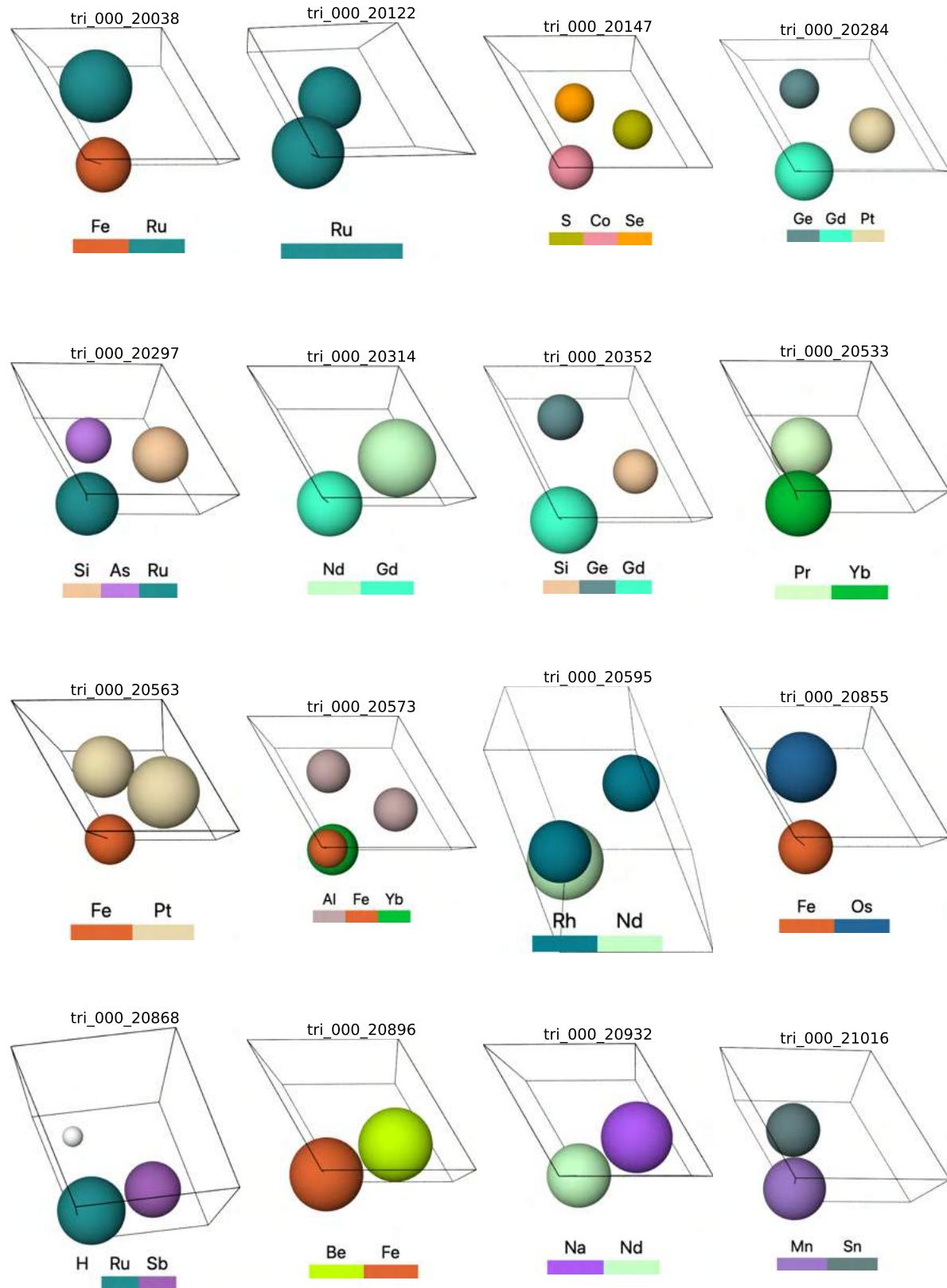


Figure S35. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

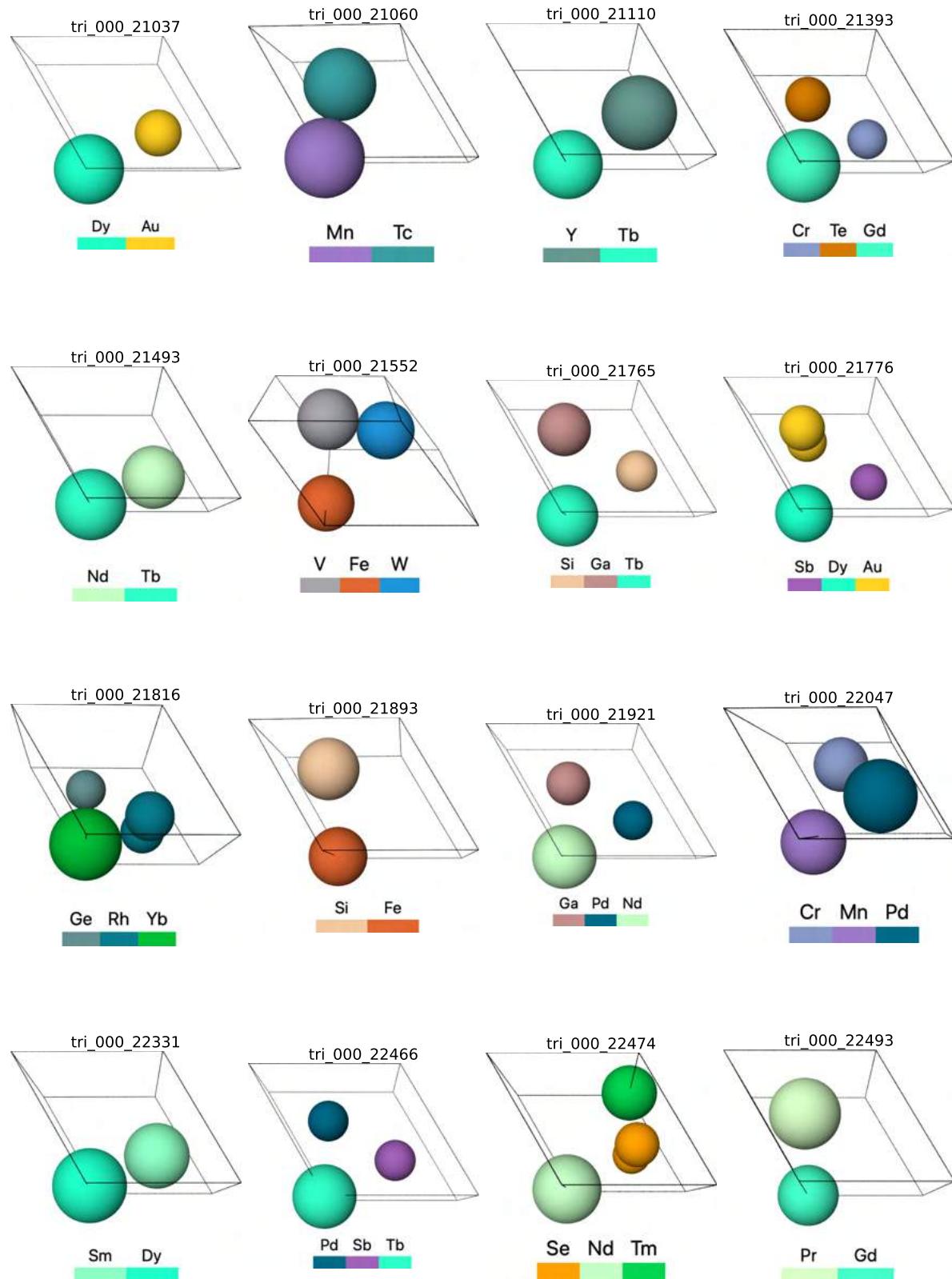


Figure S36. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

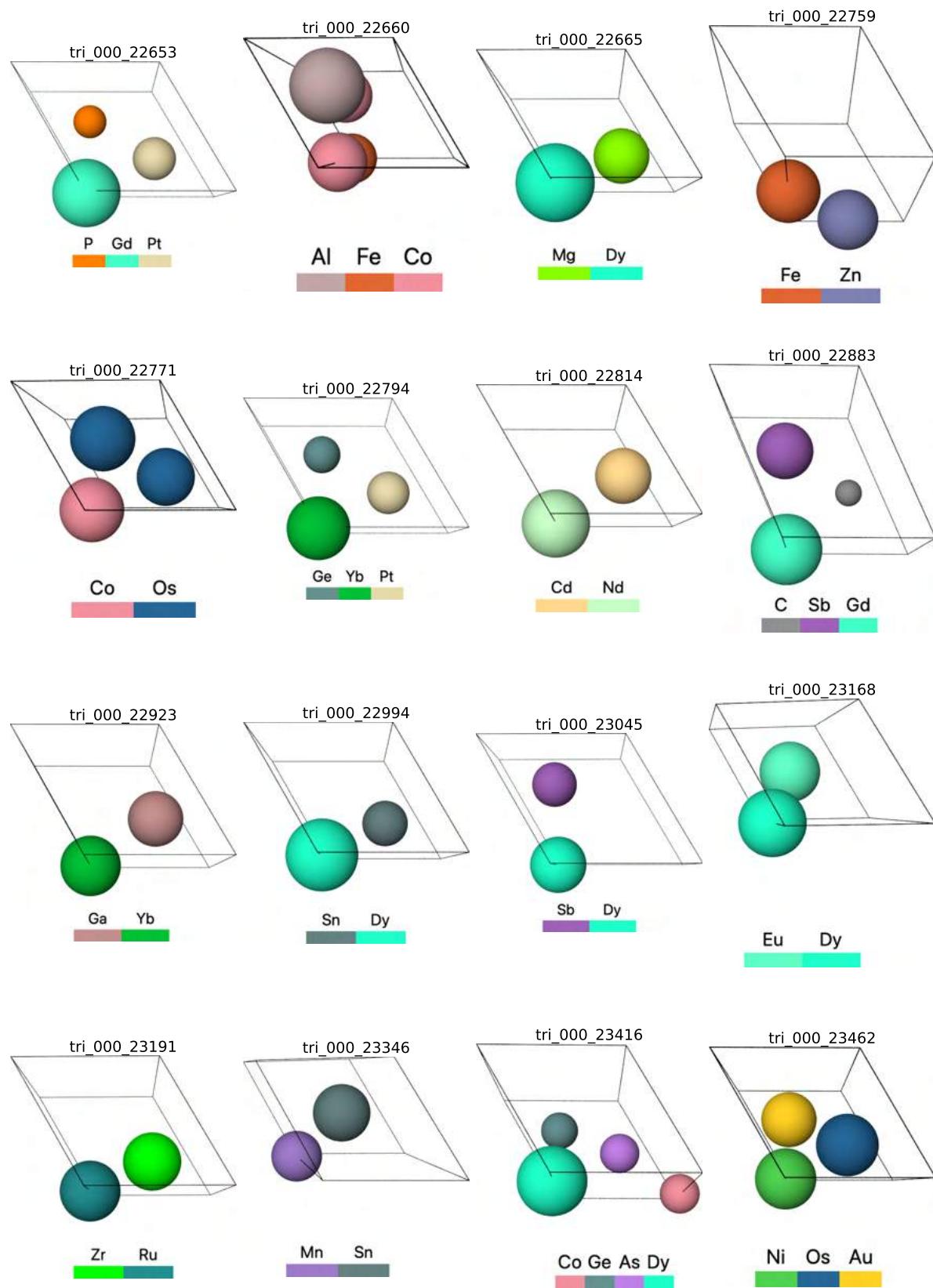


Figure S37. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

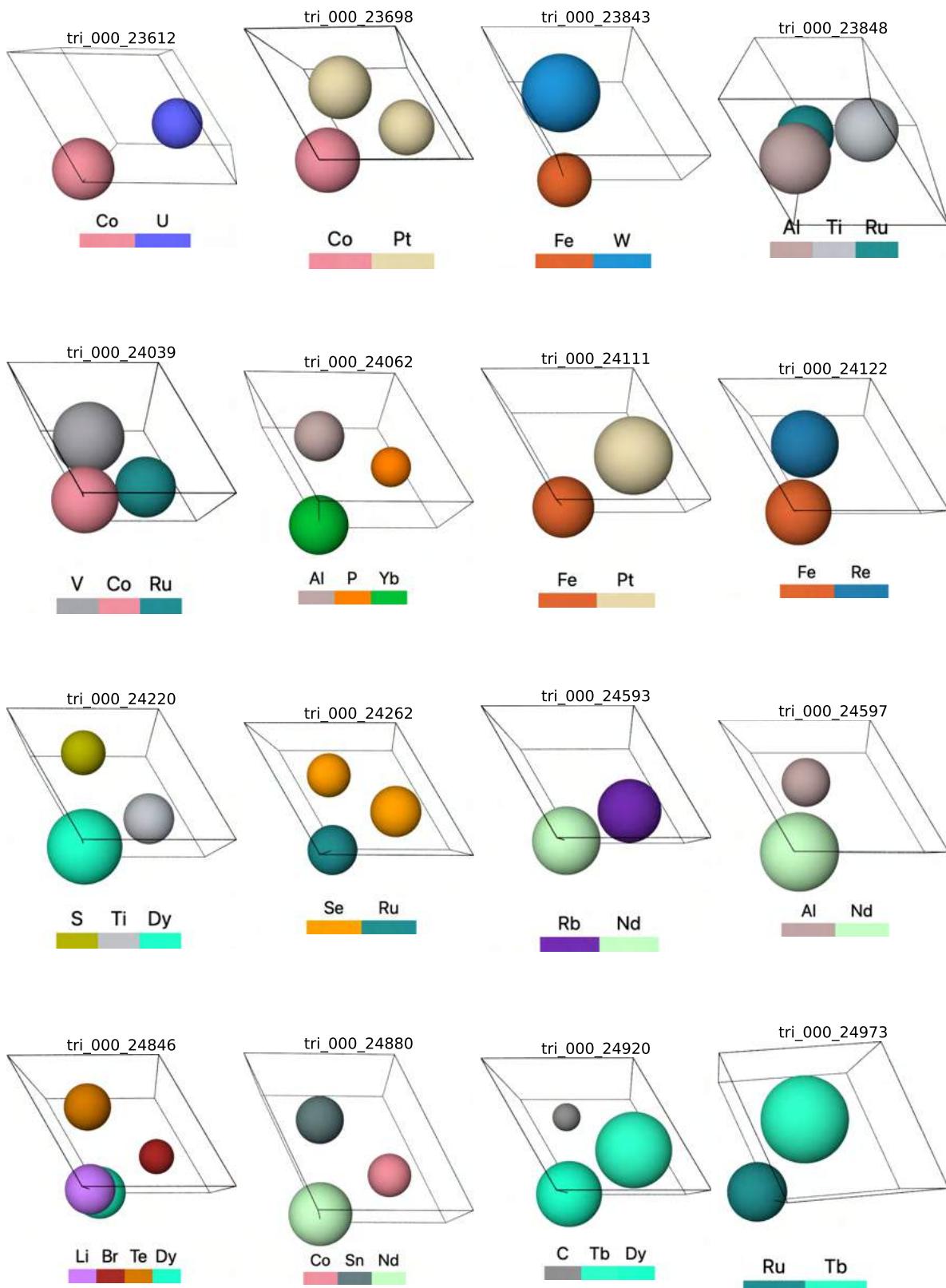


Figure S38. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

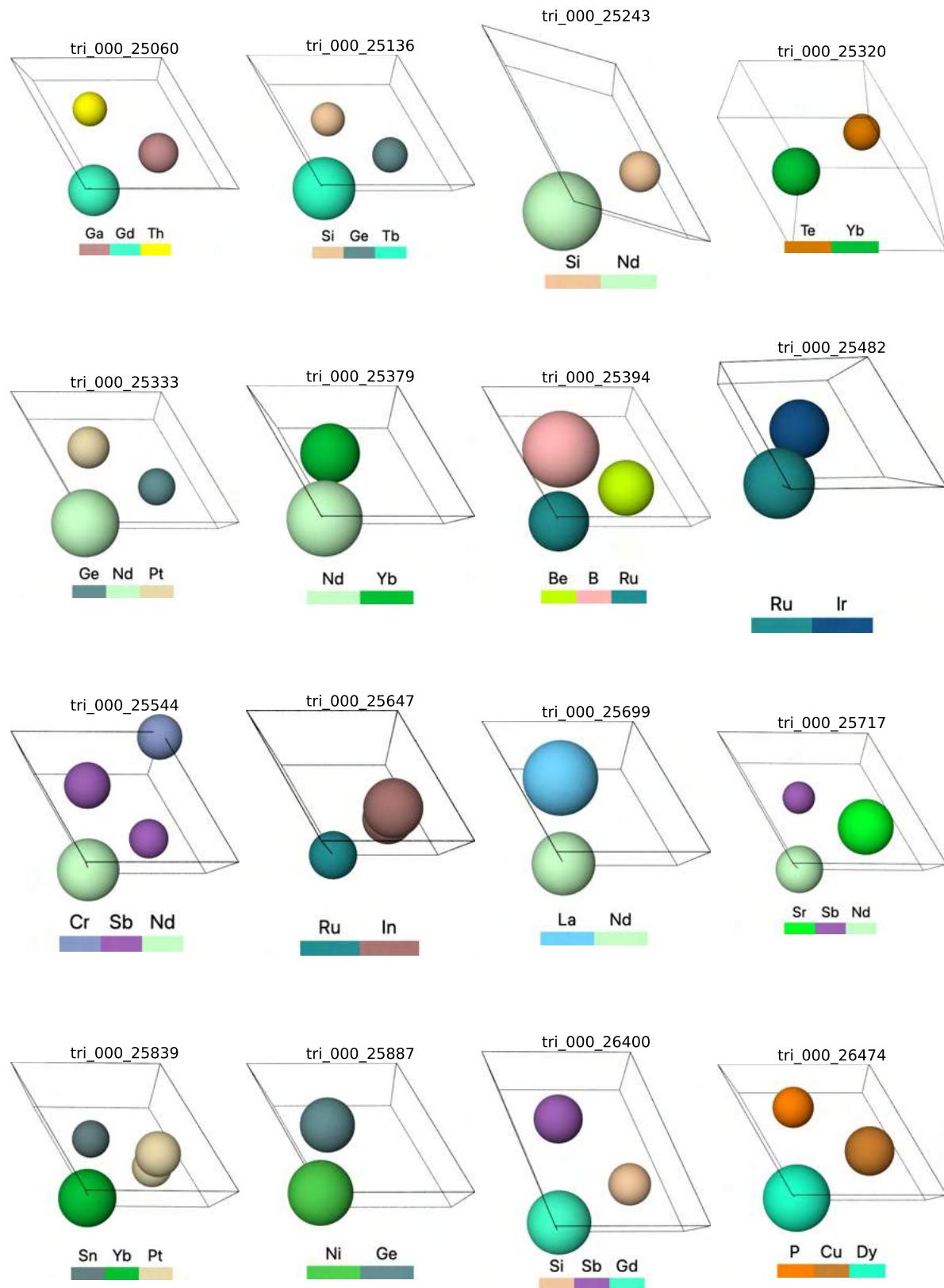


Figure S39. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

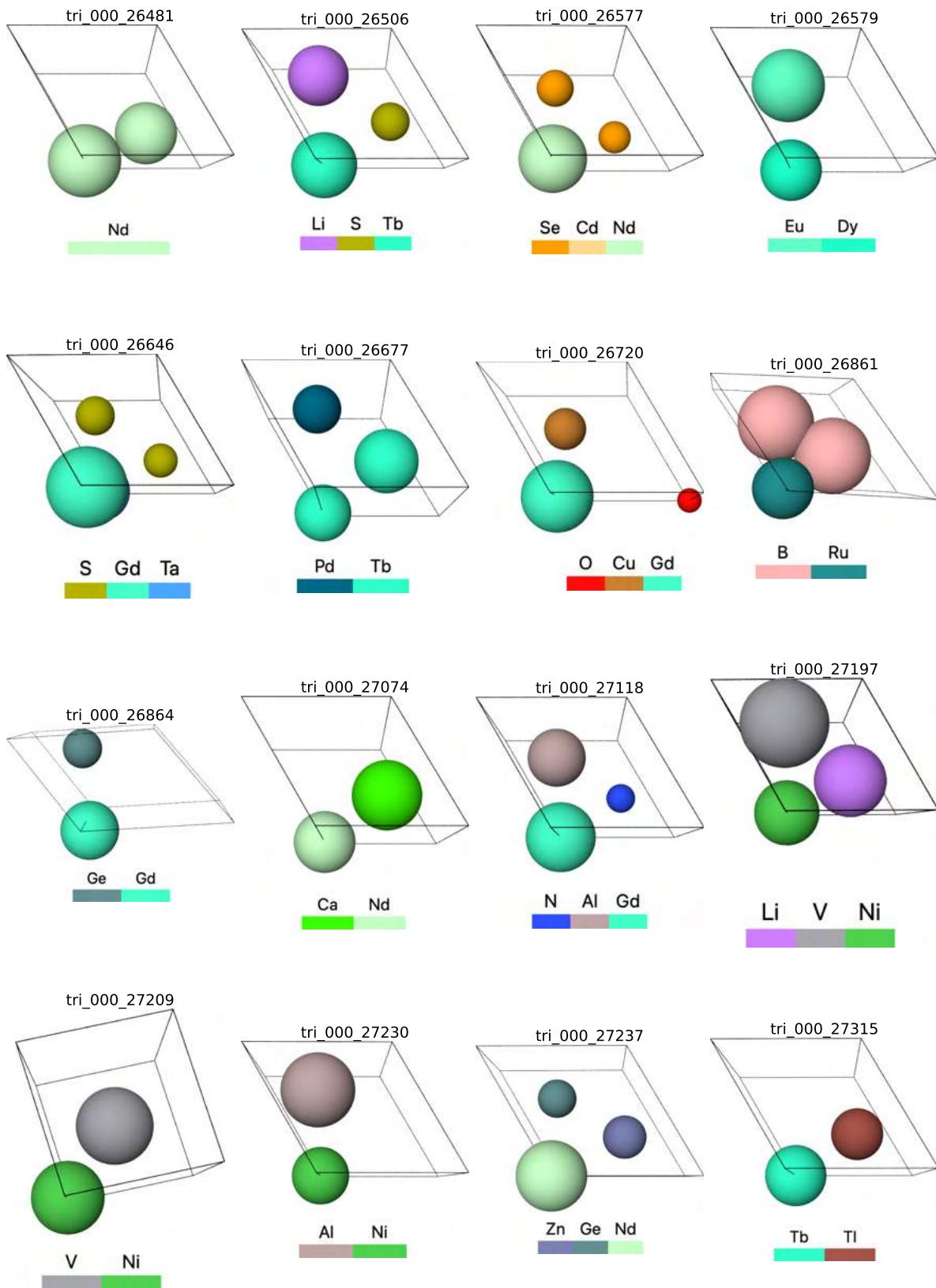


Figure S40. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

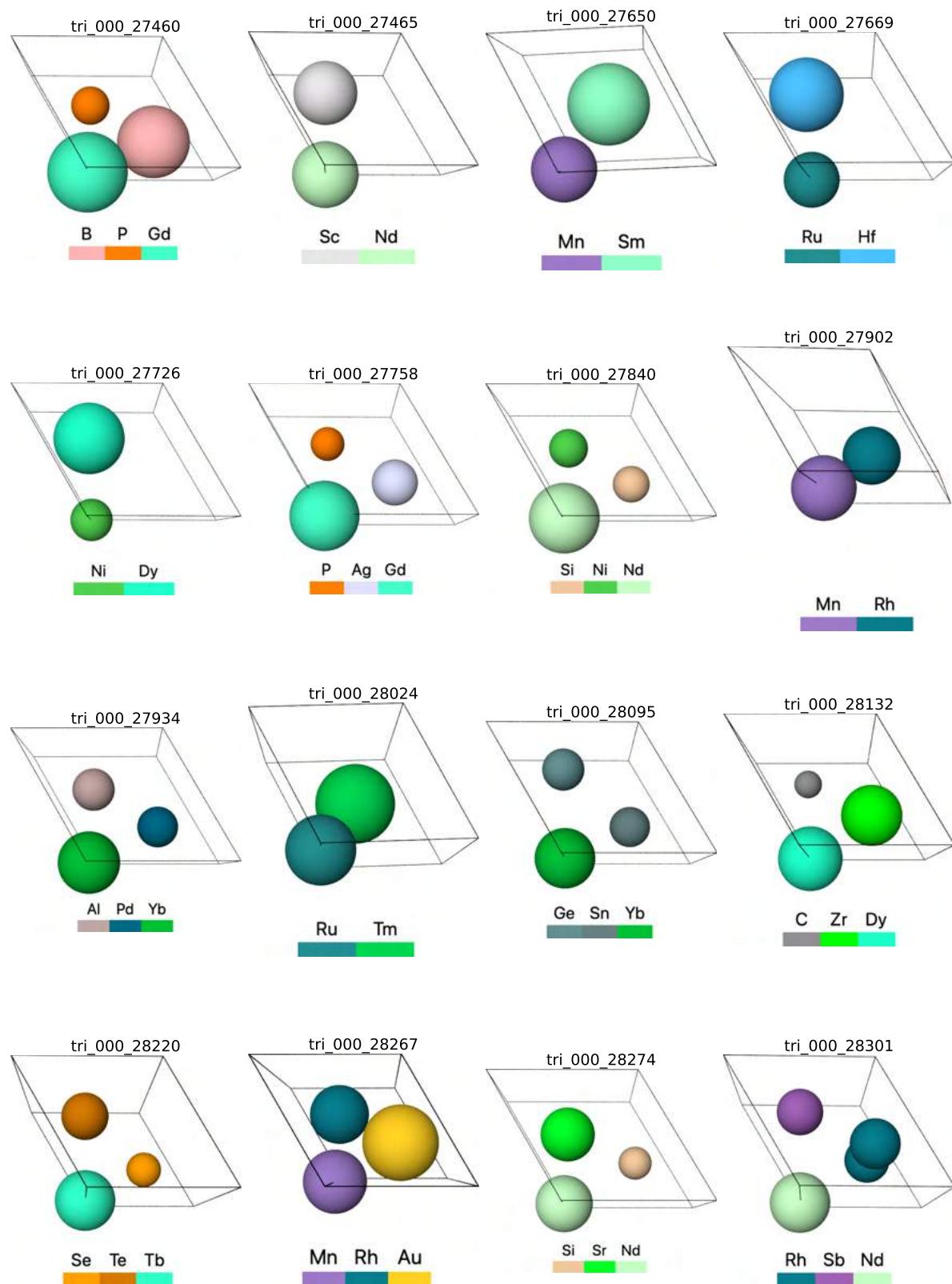


Figure S41. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

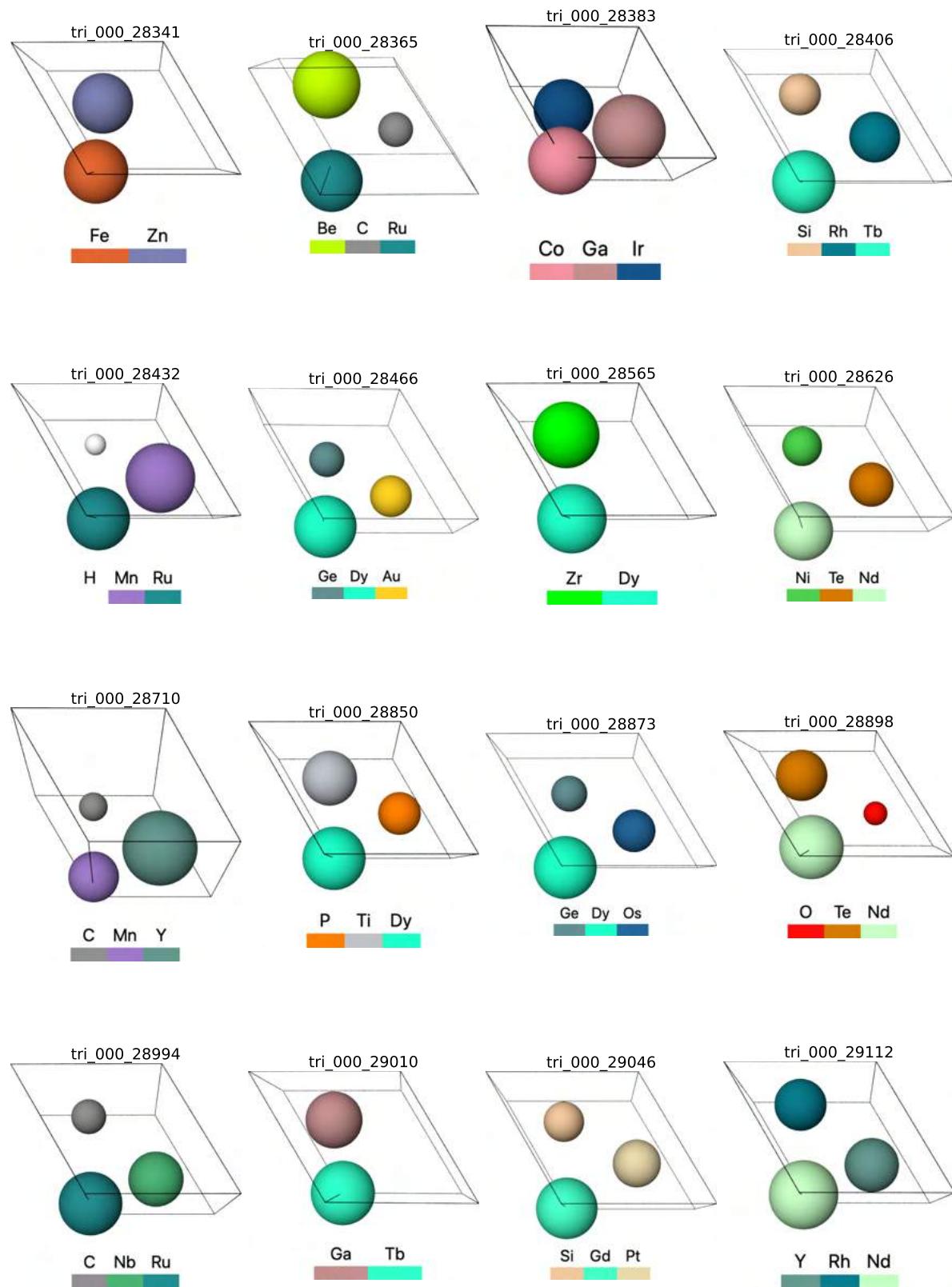


Figure S42. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

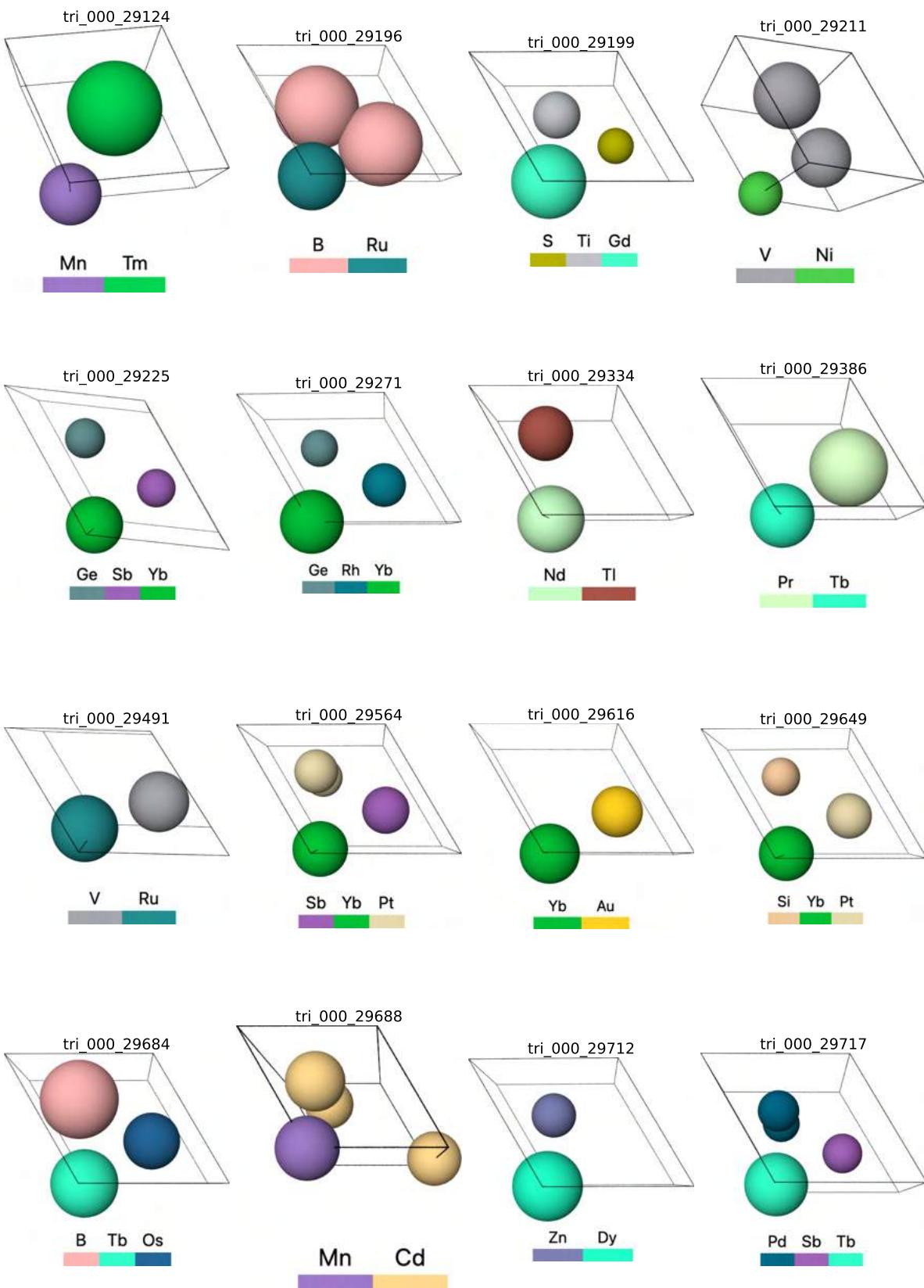


Figure S43. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

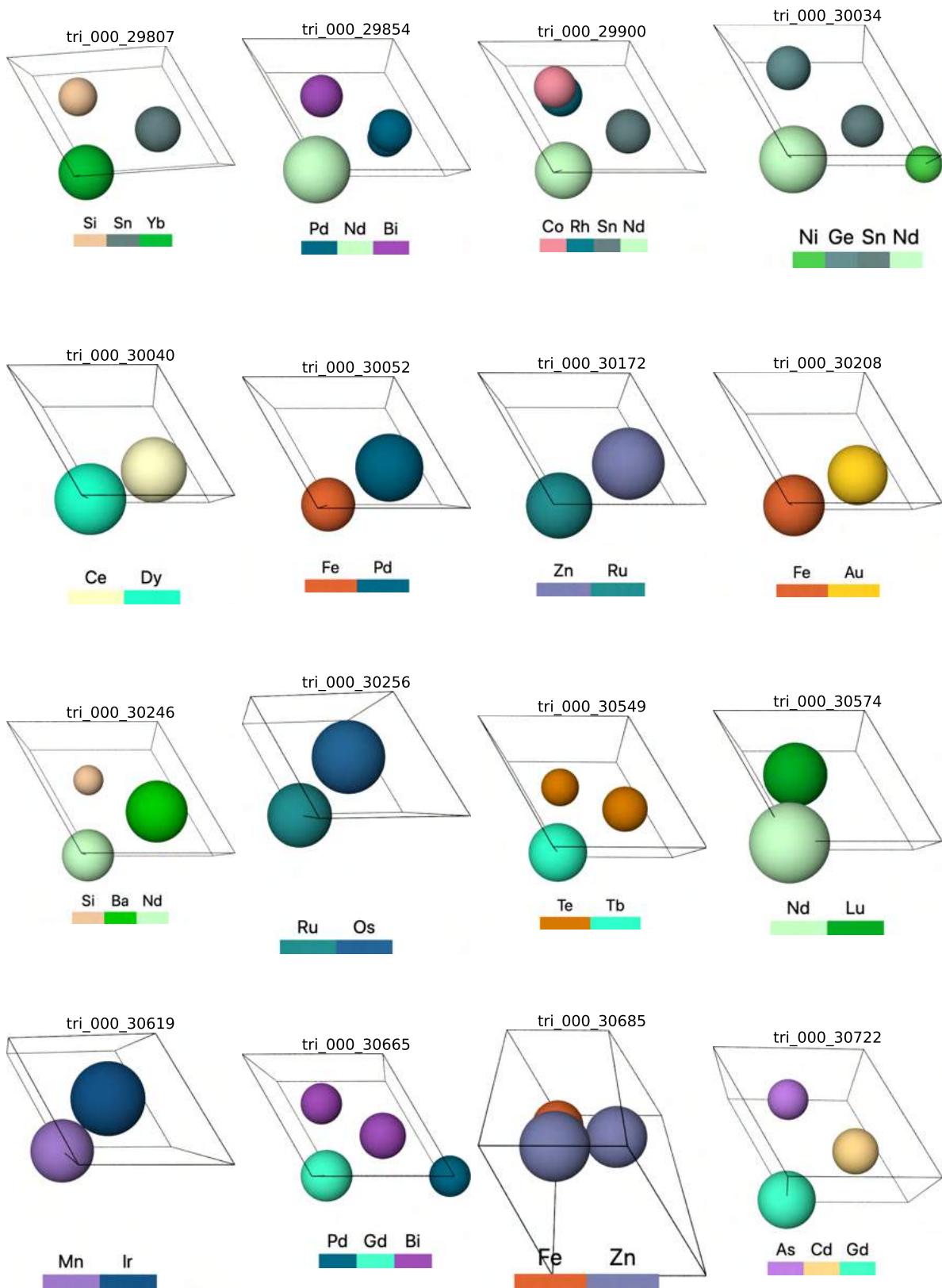


Figure S44. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

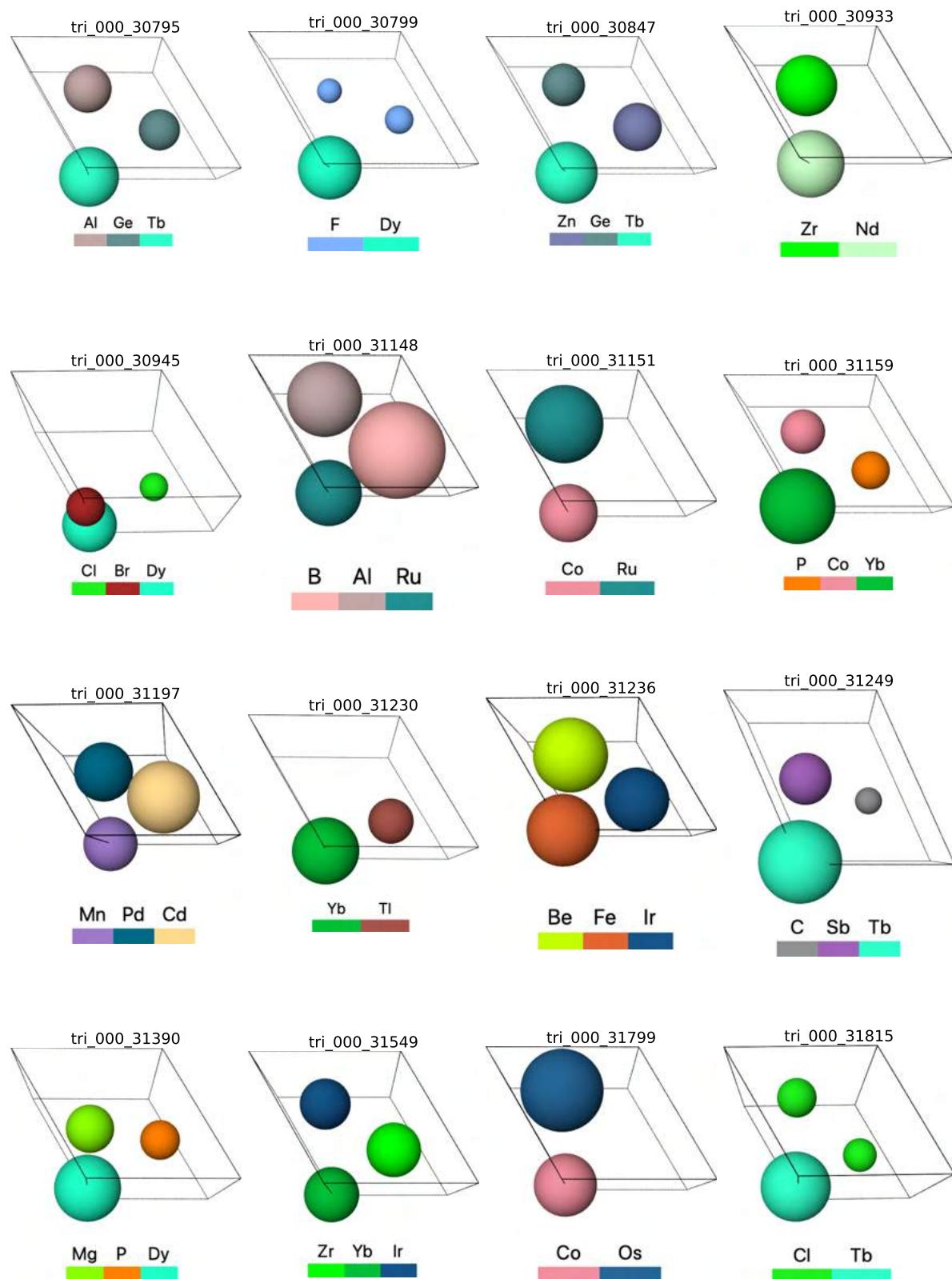


Figure S45. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

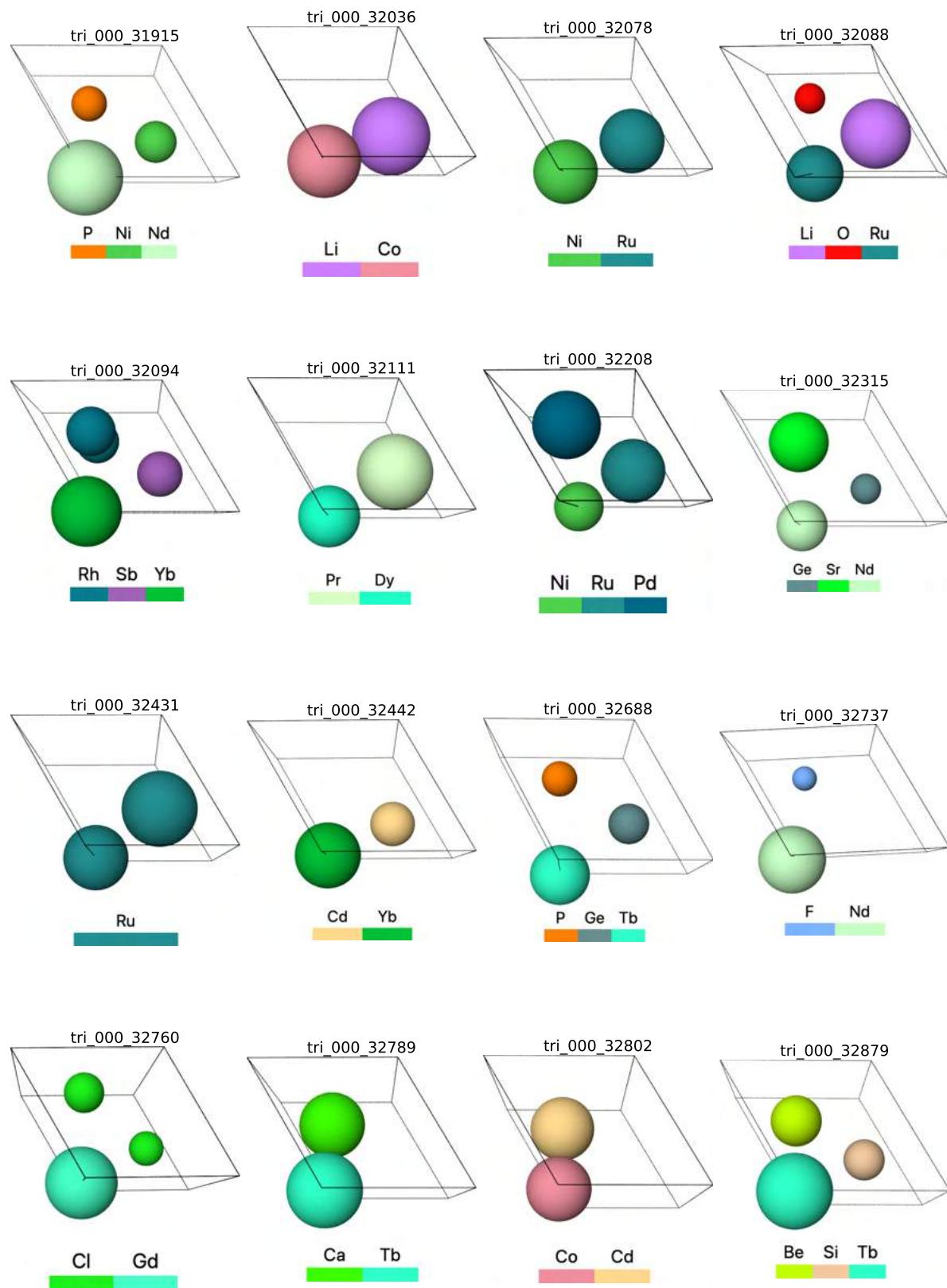


Figure S46. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

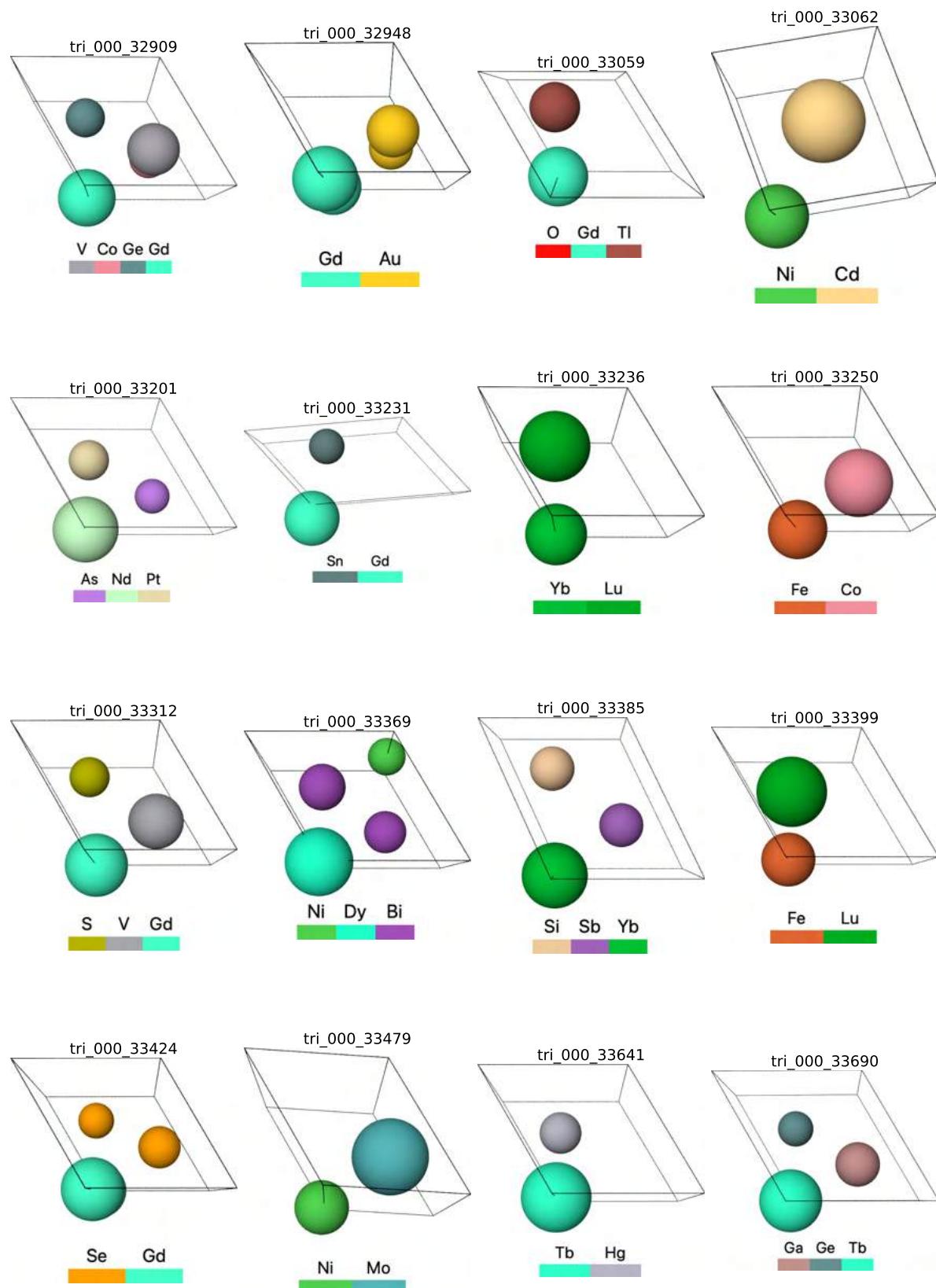


Figure S47. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

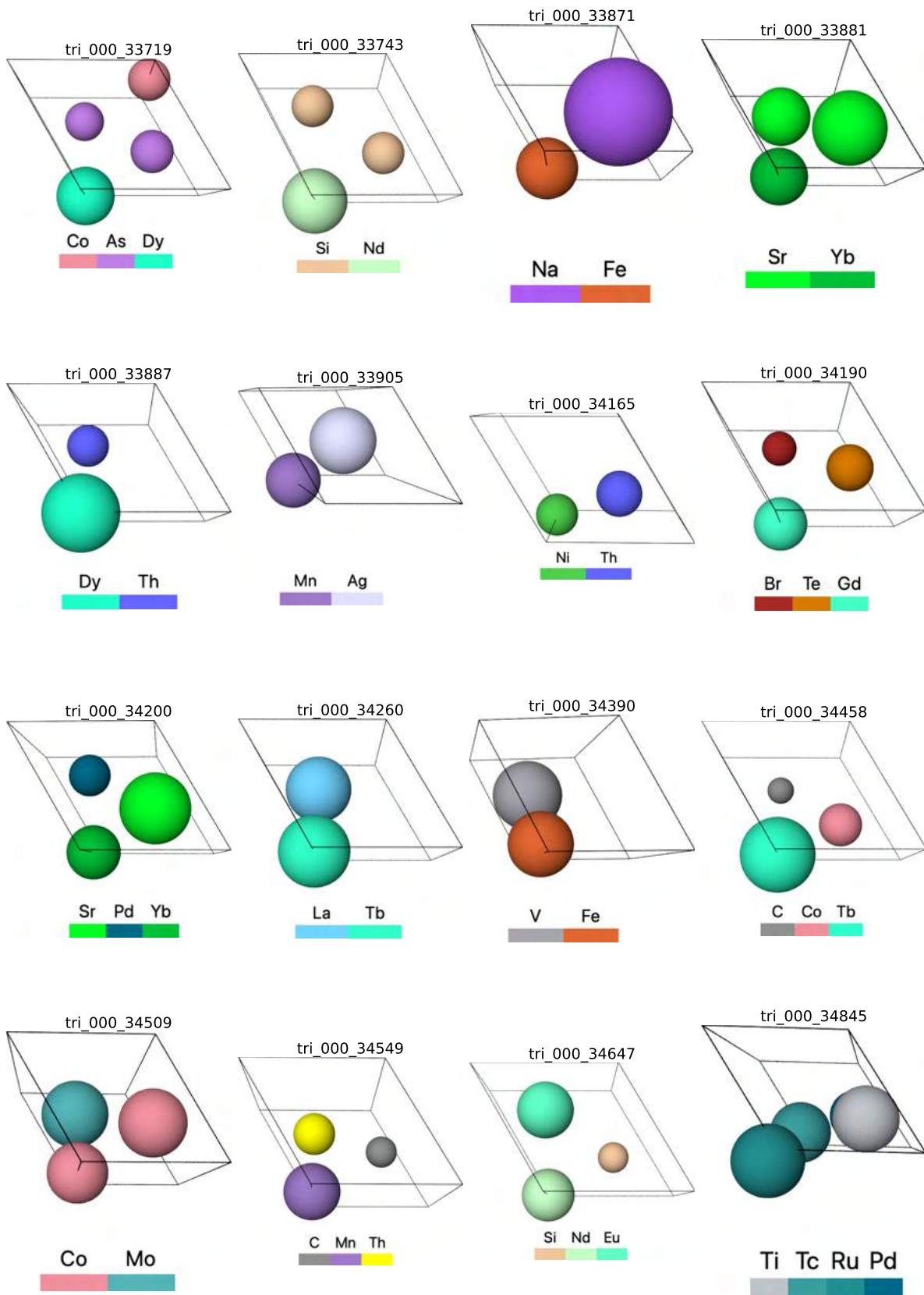


Figure S48. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

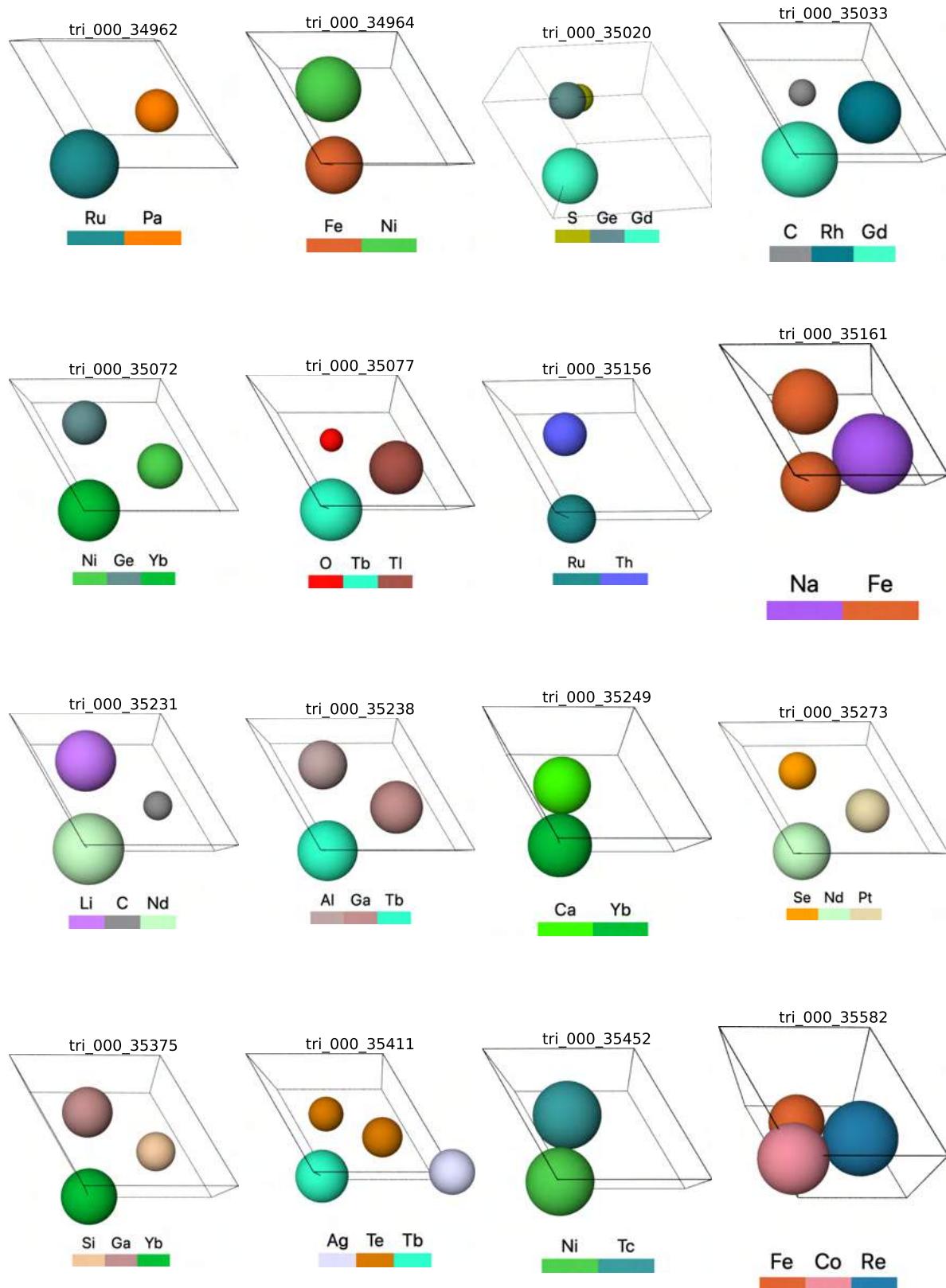


Figure S49. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

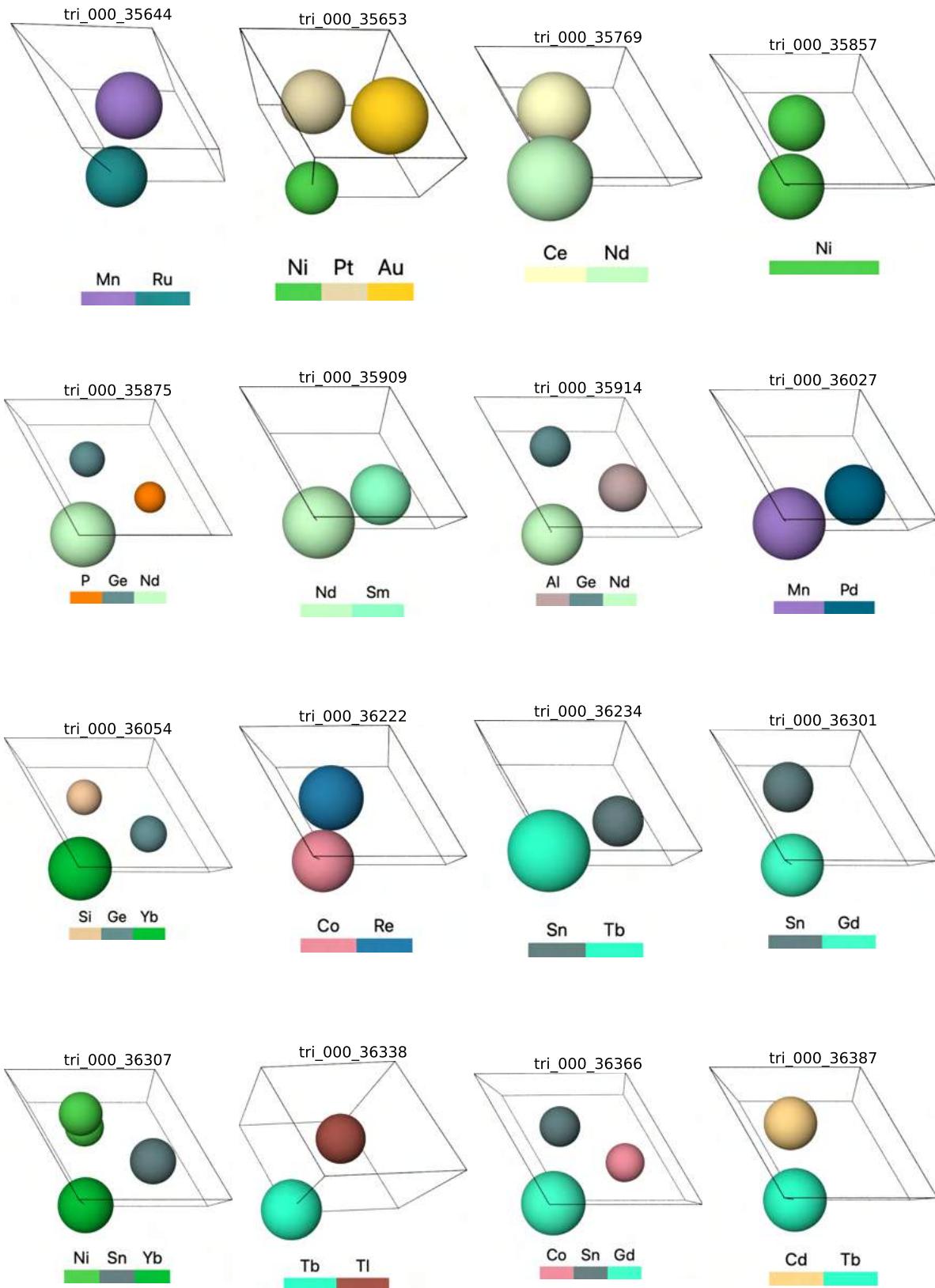


Figure S50. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

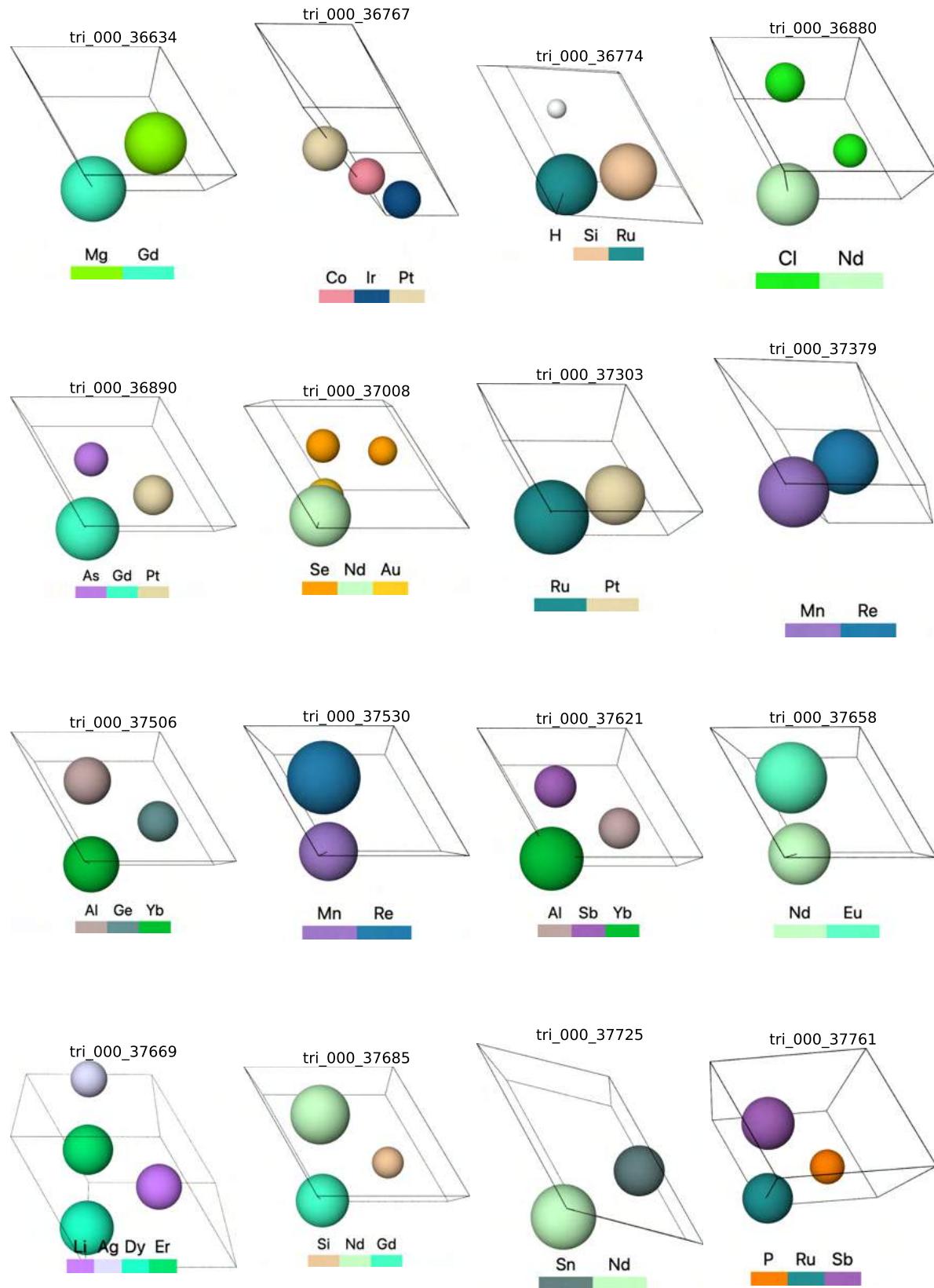


Figure S51. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

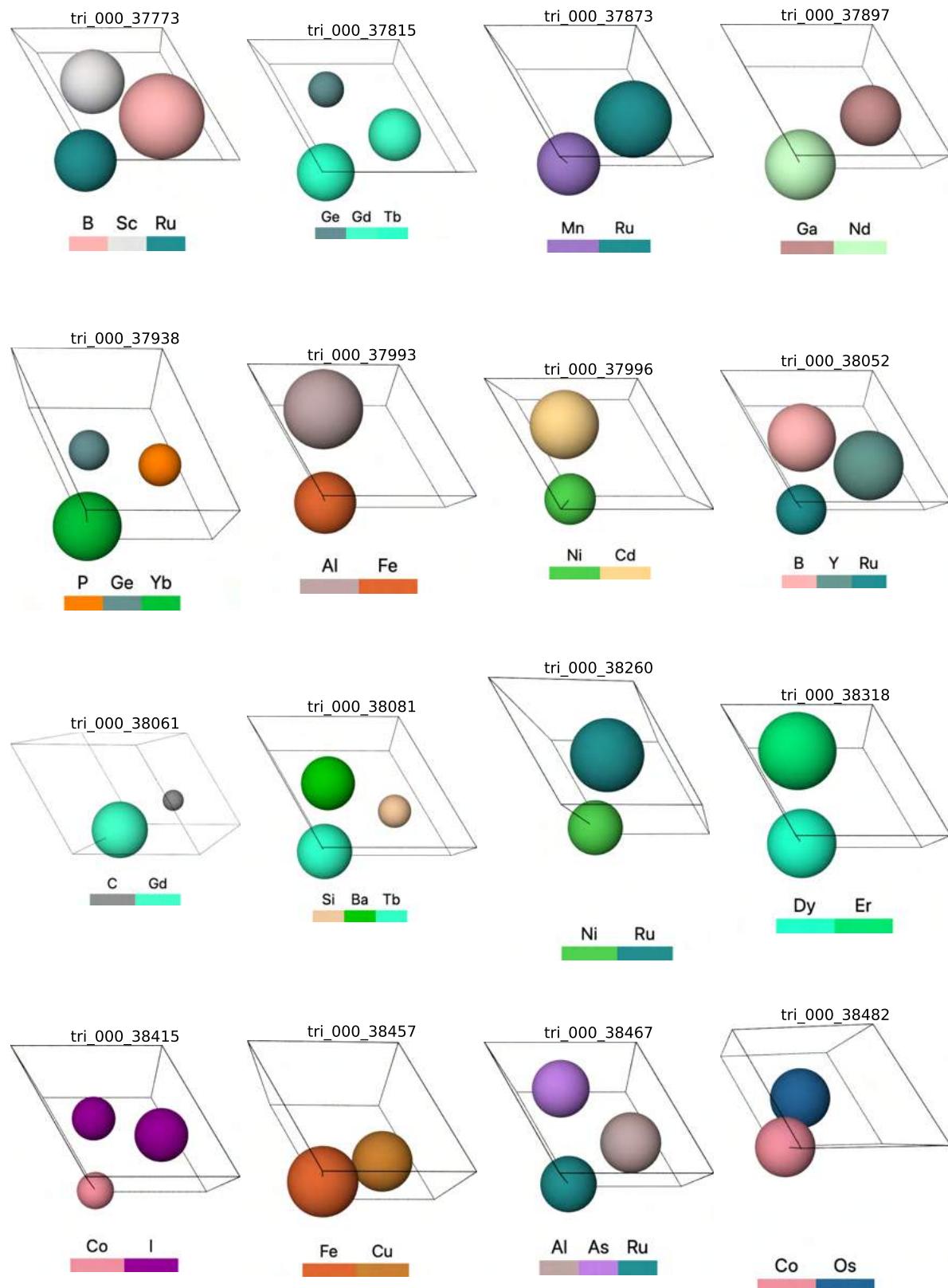


Figure S52. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

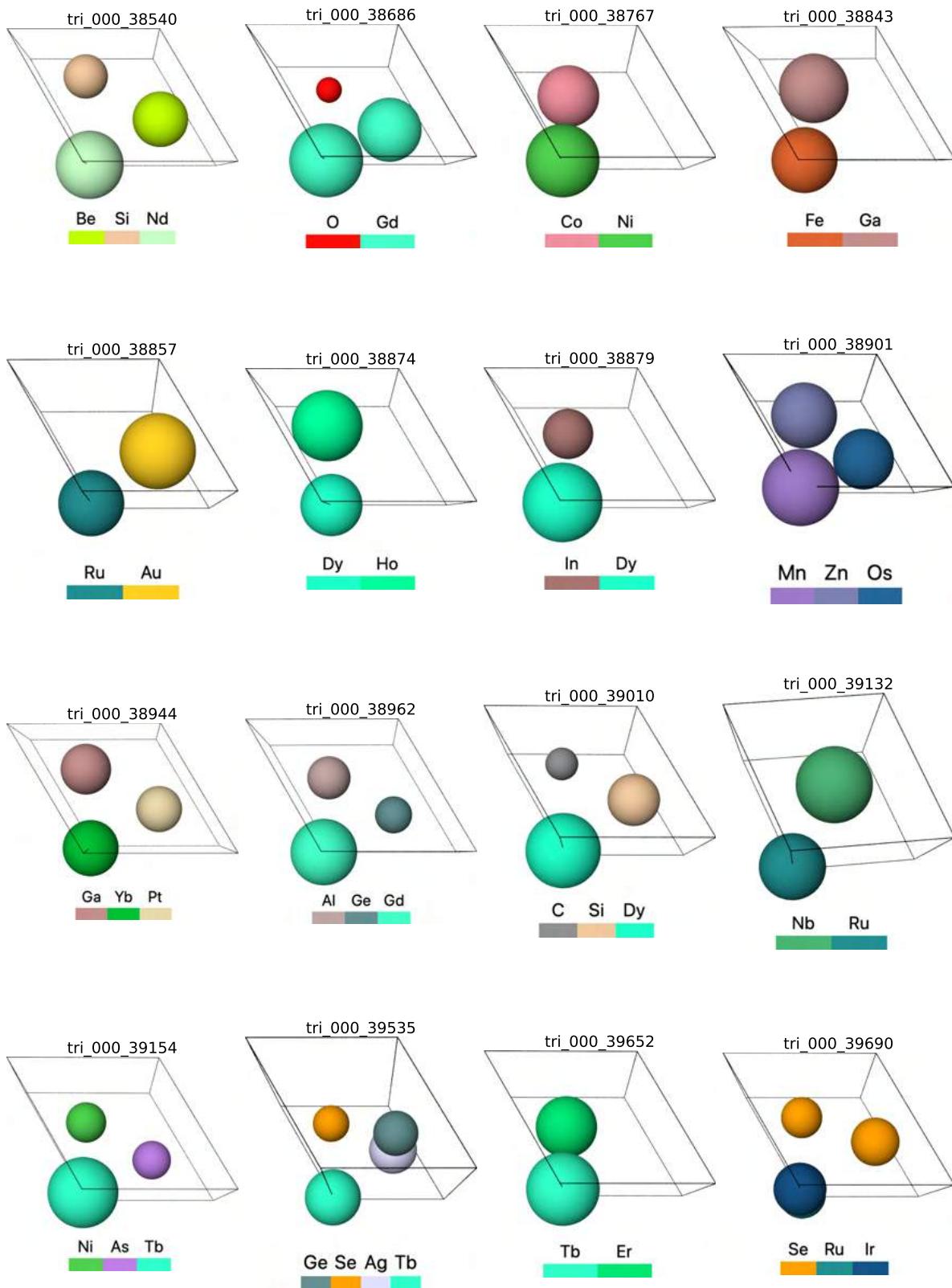


Figure S53. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

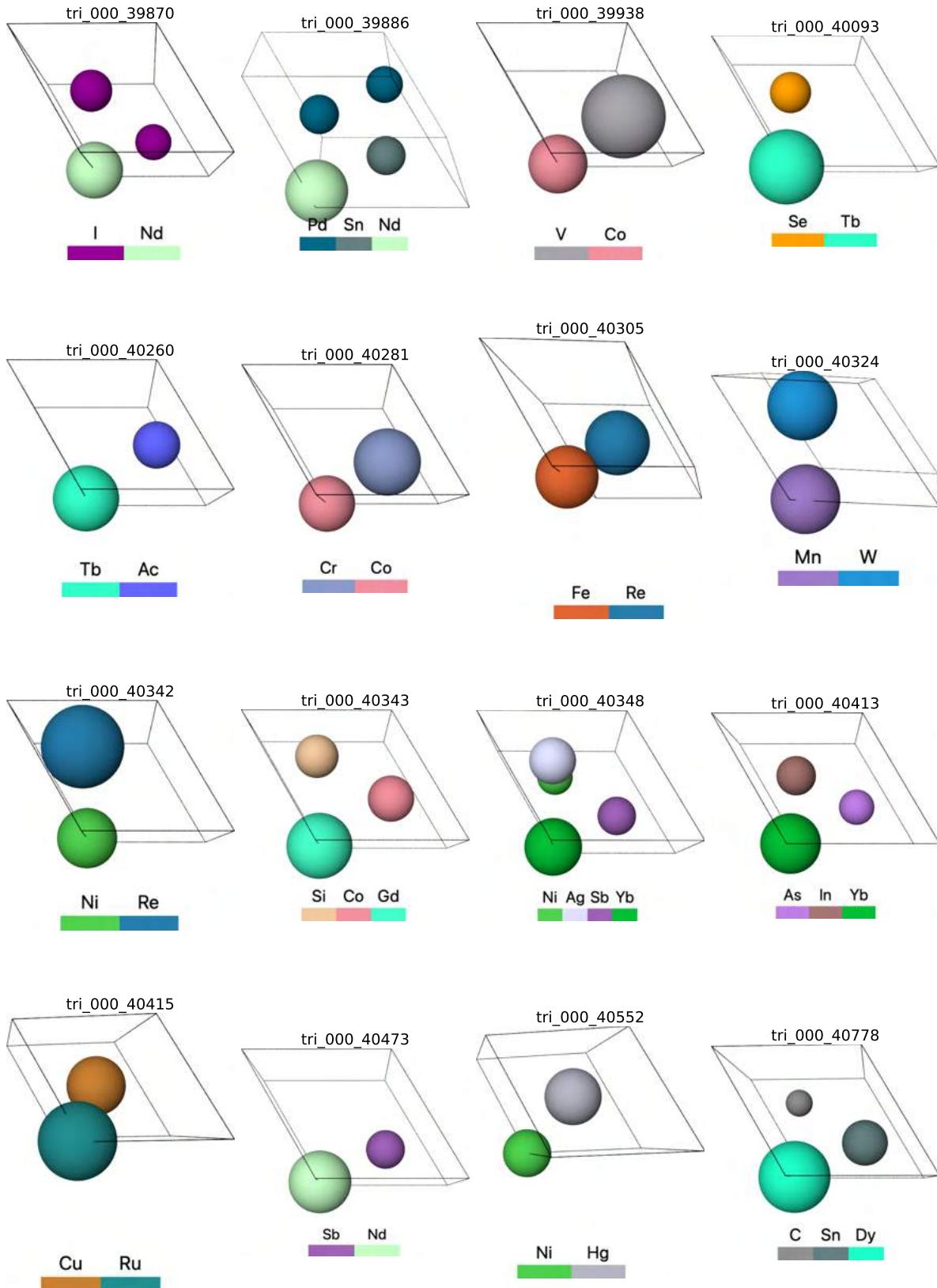


Figure S54. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

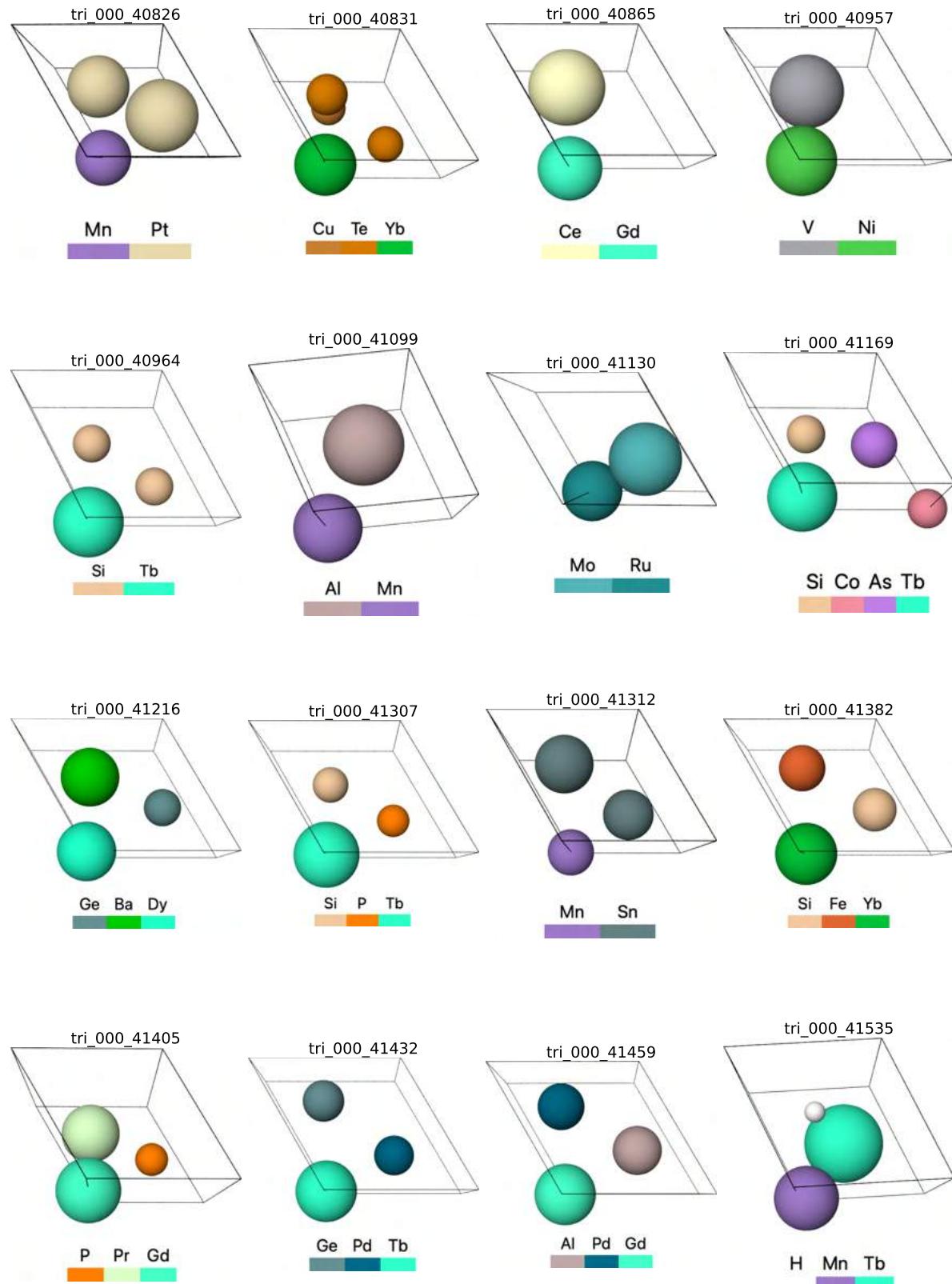


Figure S55. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

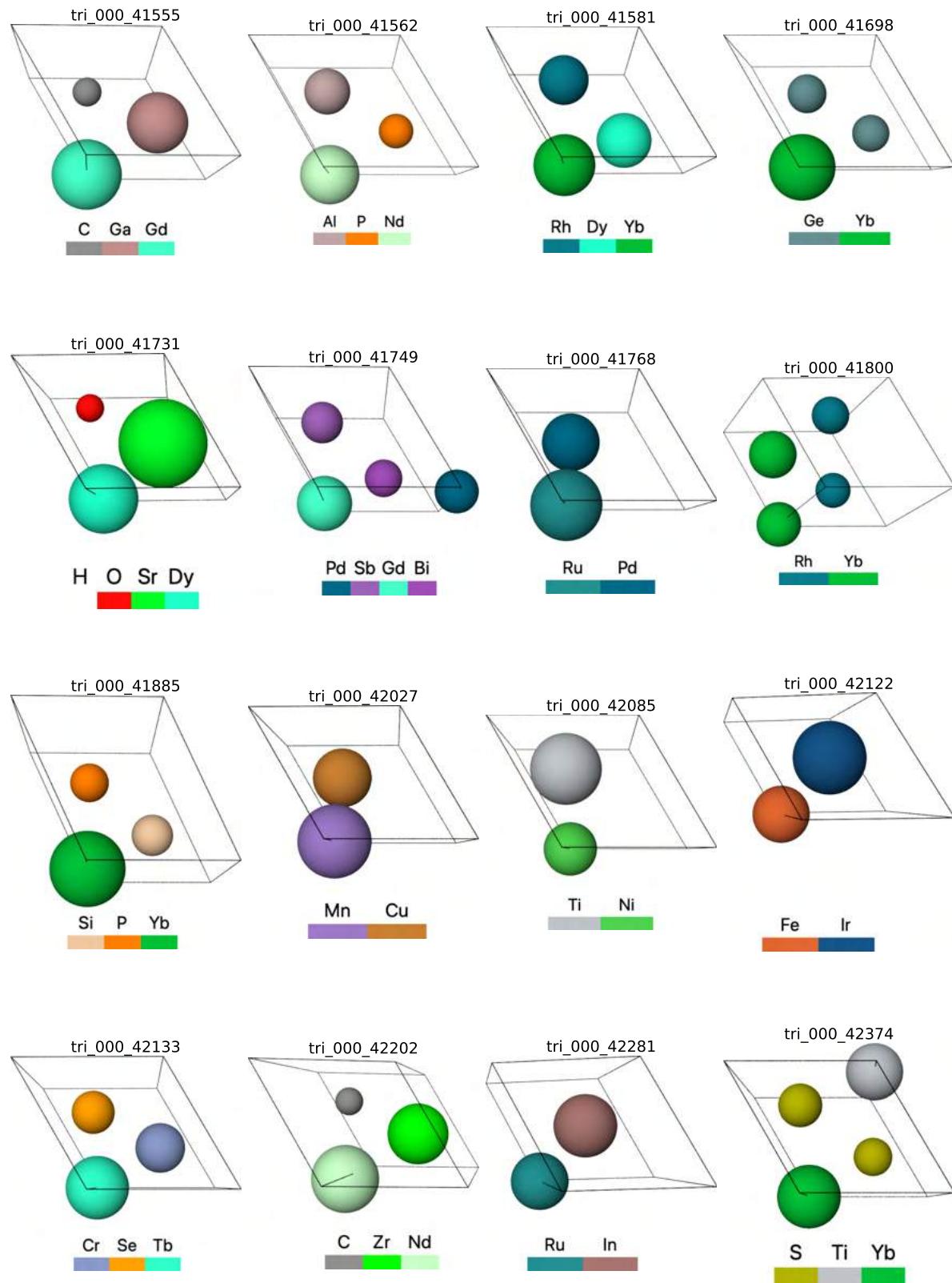


Figure S56. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

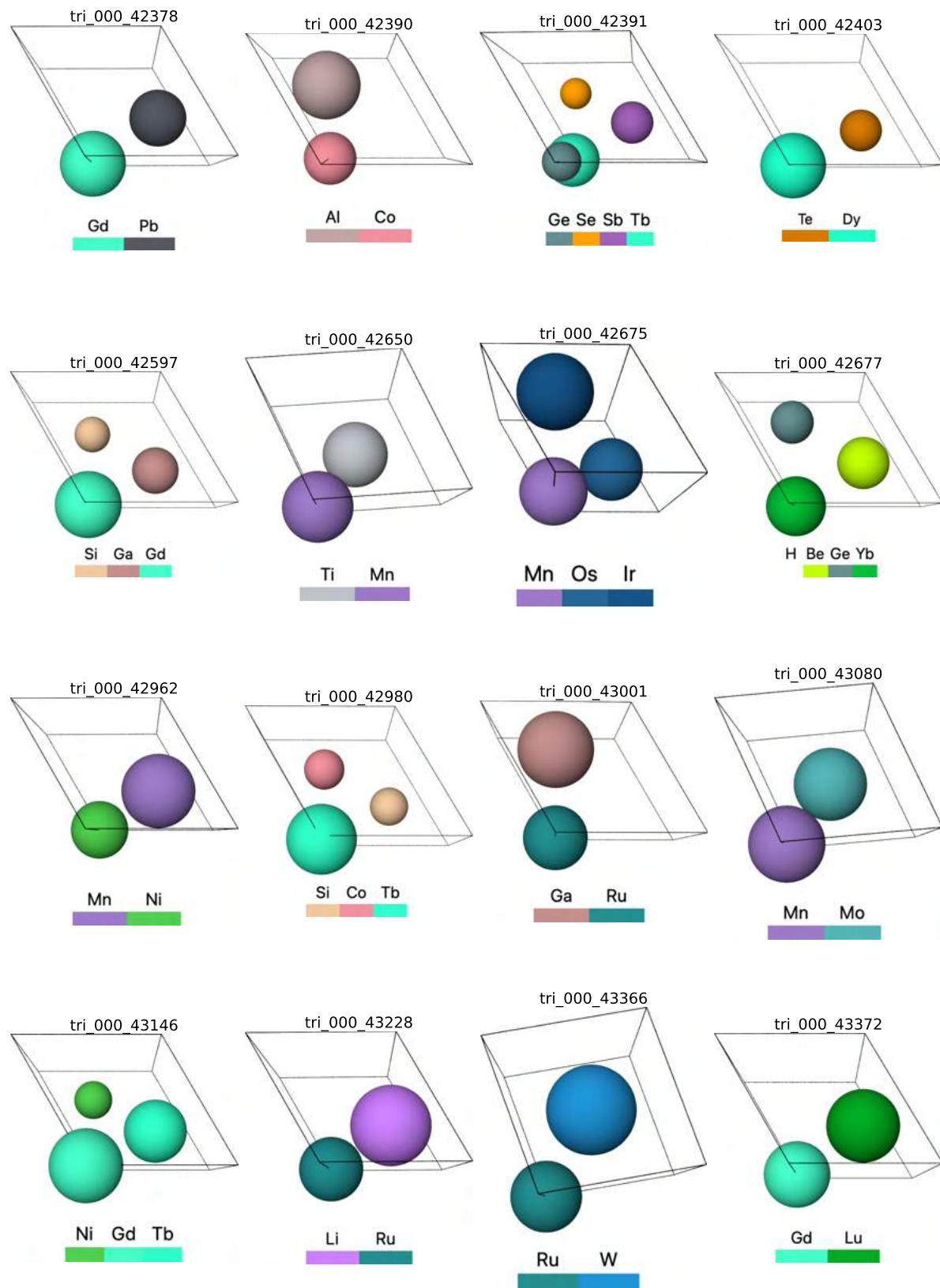


Figure S57. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

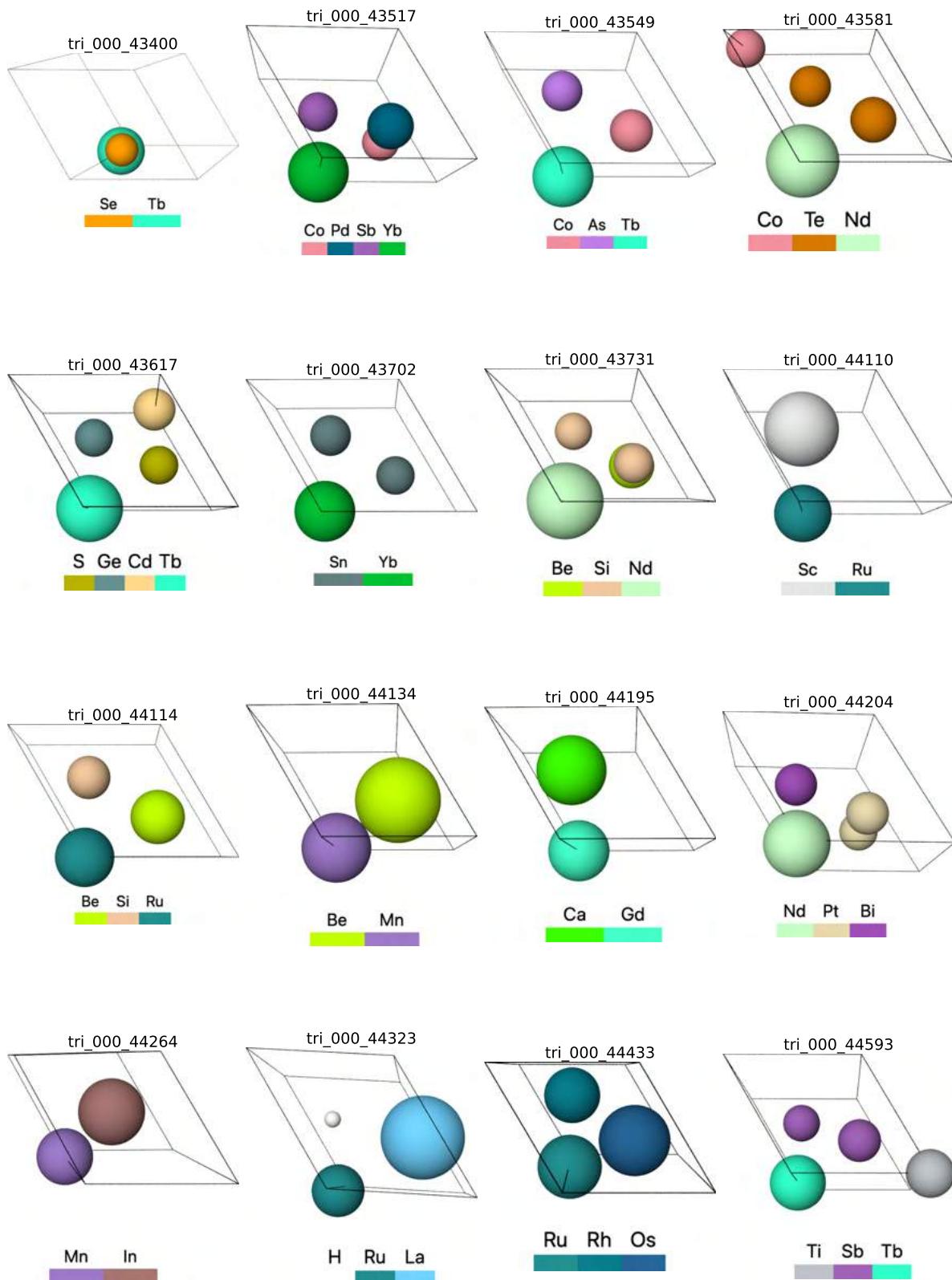


Figure S58. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

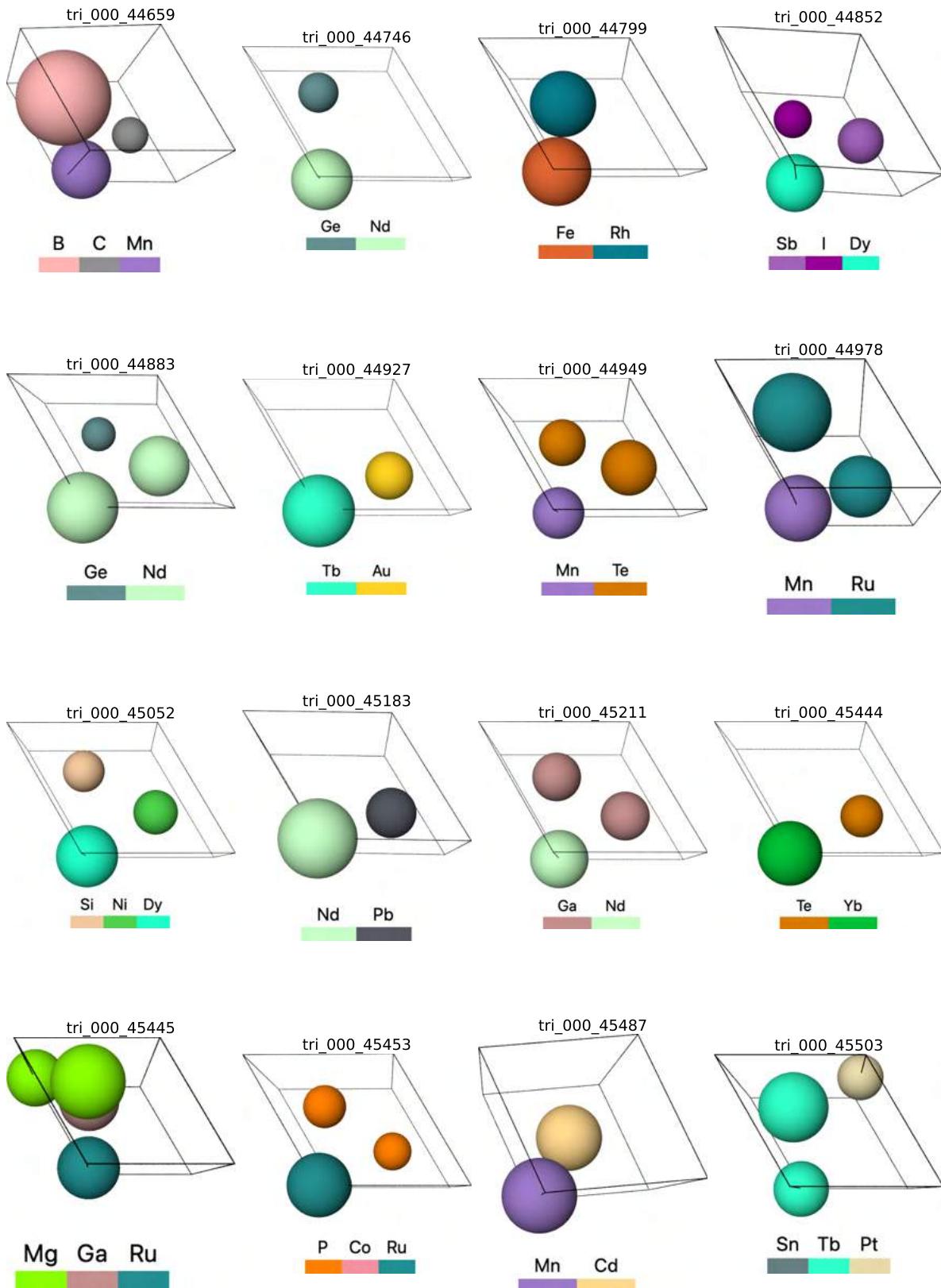


Figure S59. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

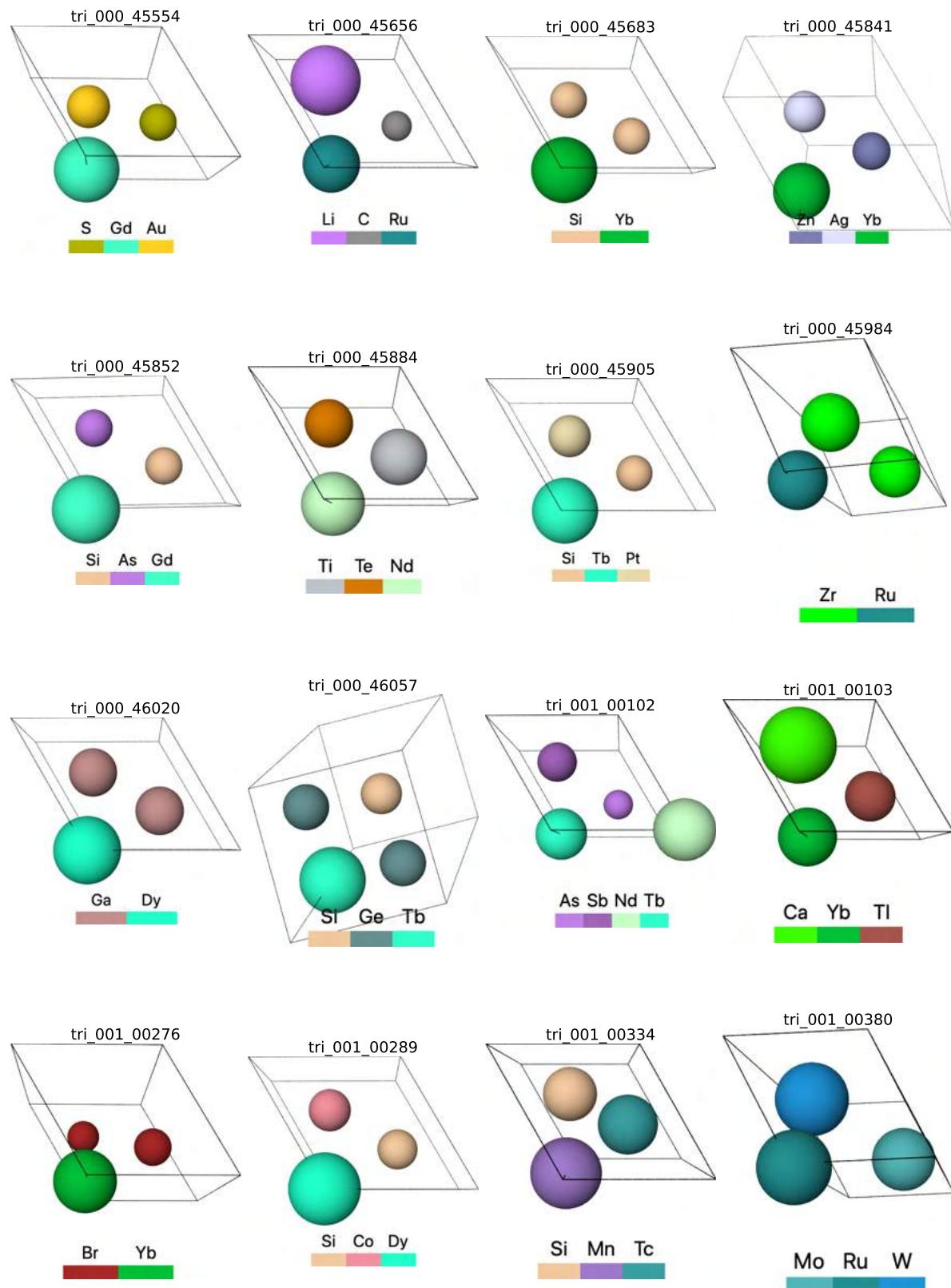


Figure S60. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

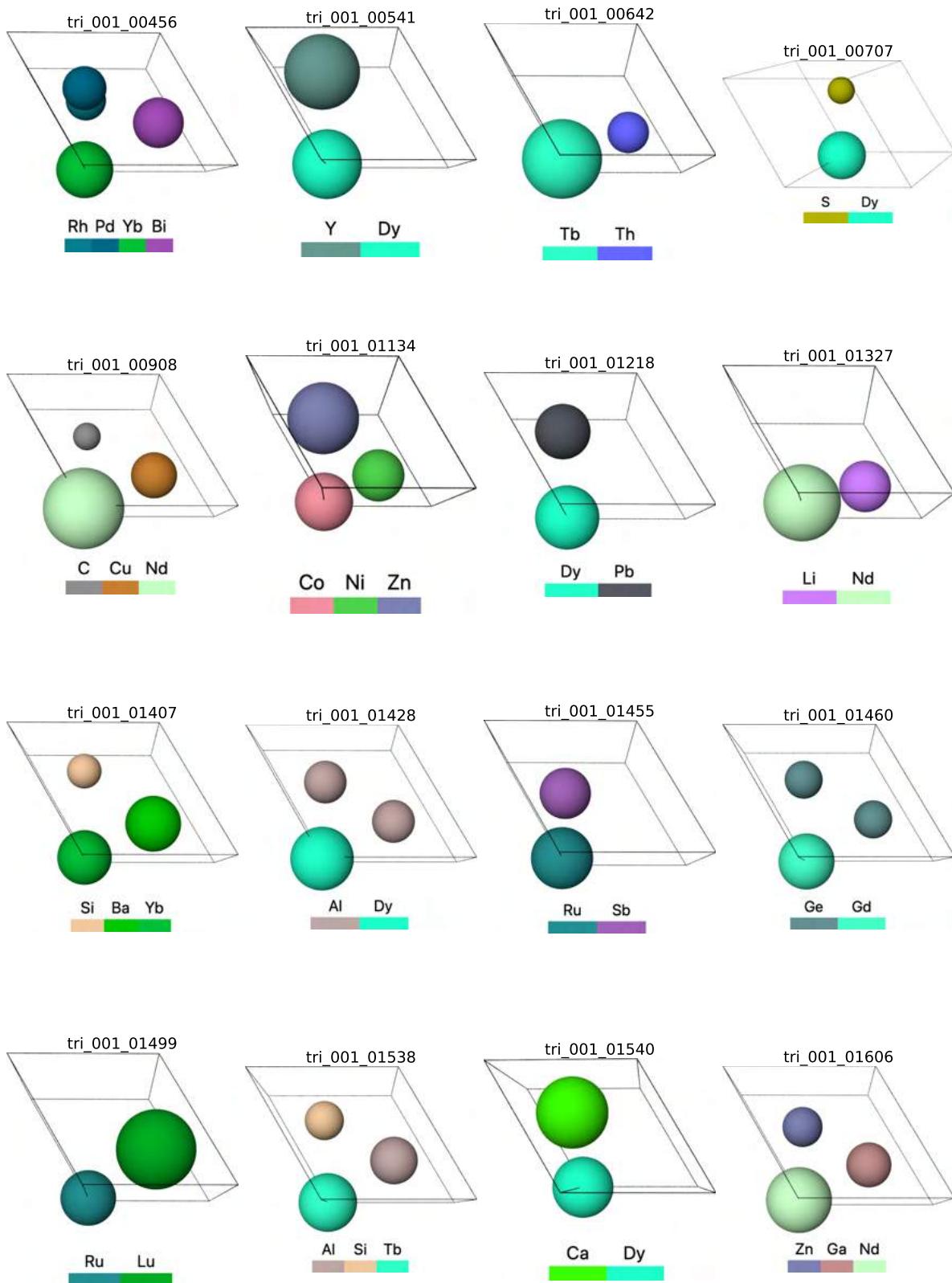


Figure S61. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

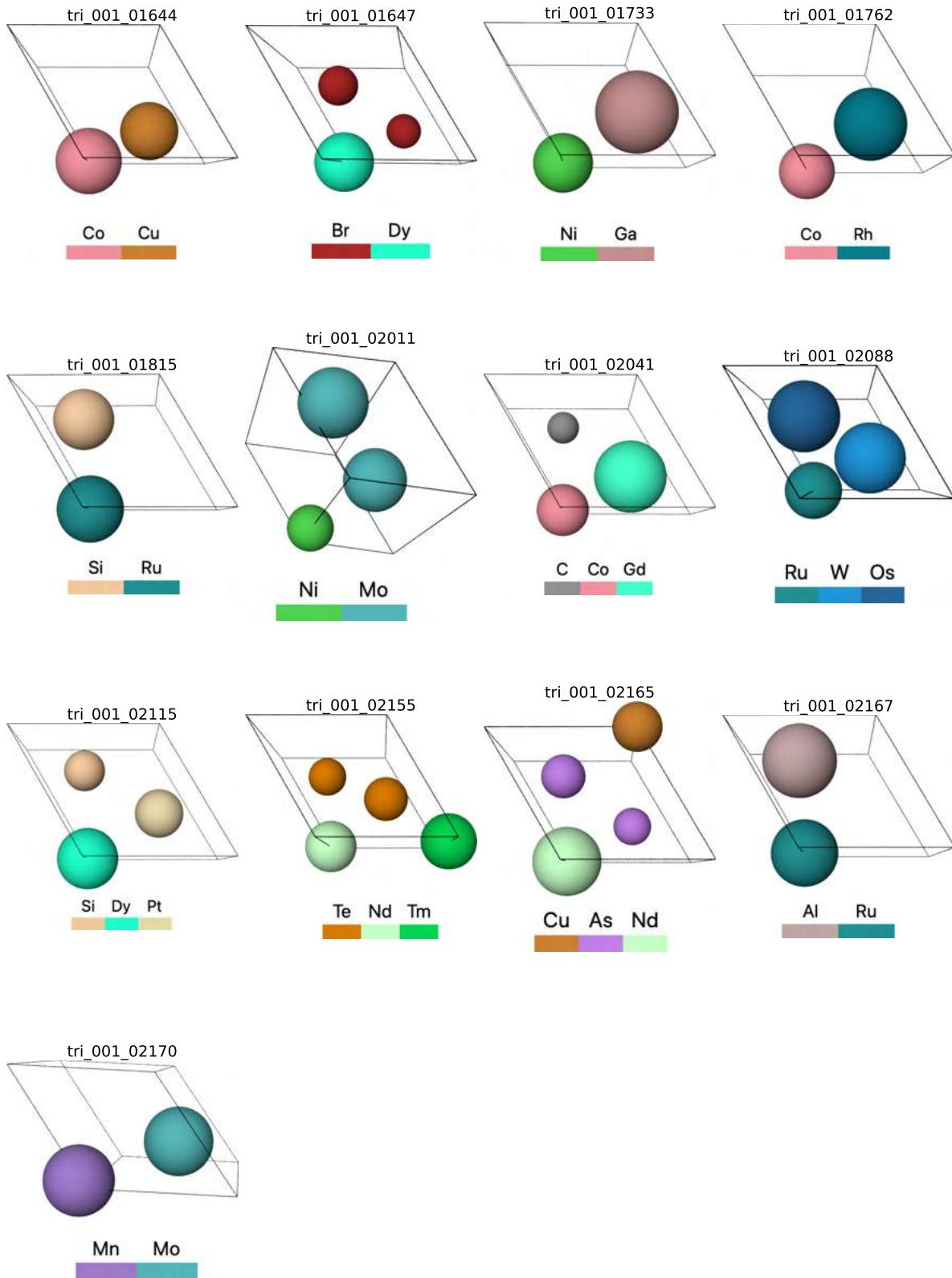


Figure S62. Generated materials with Triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

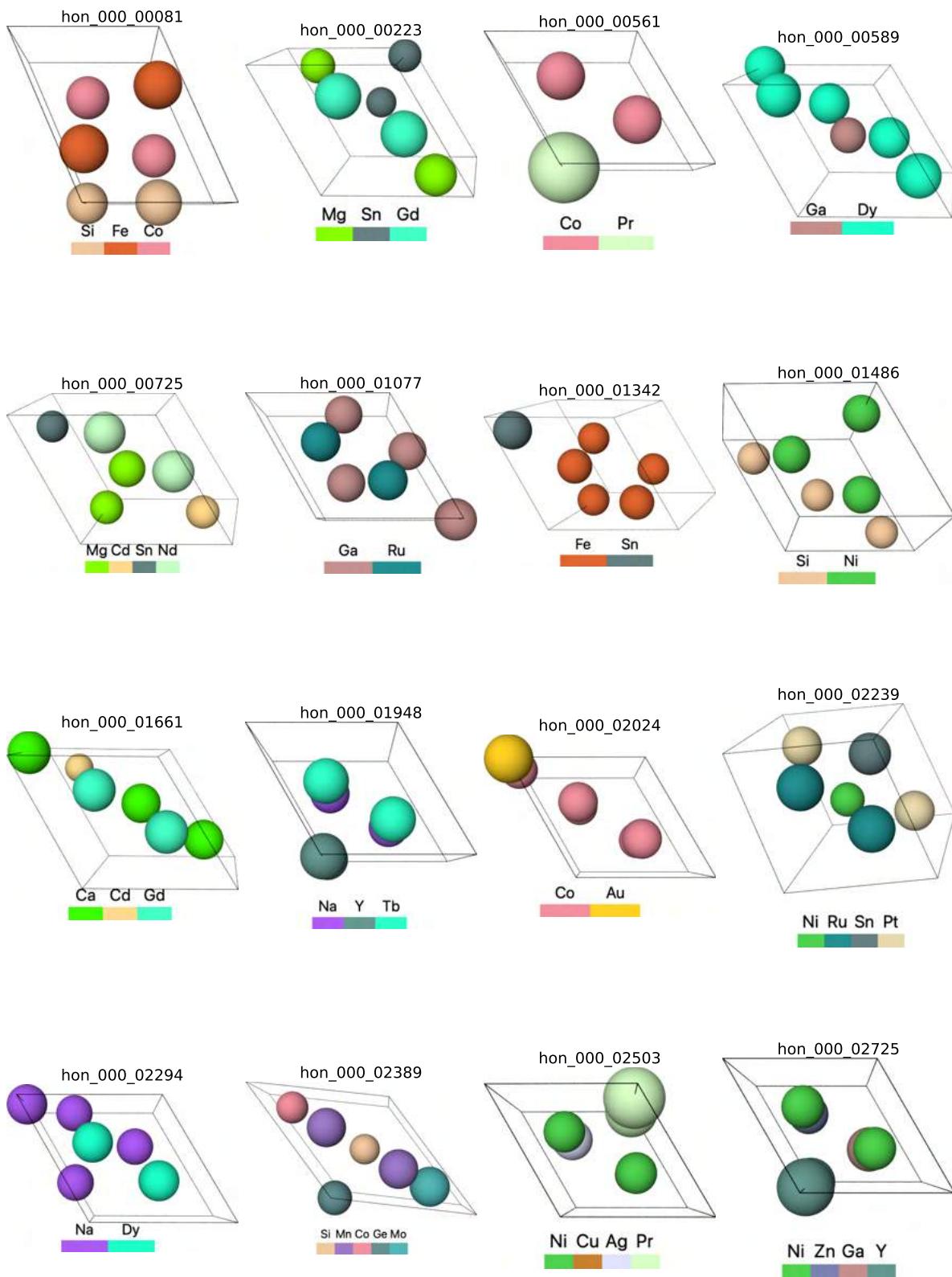


Figure S63. Generated materials with Honeycomb lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

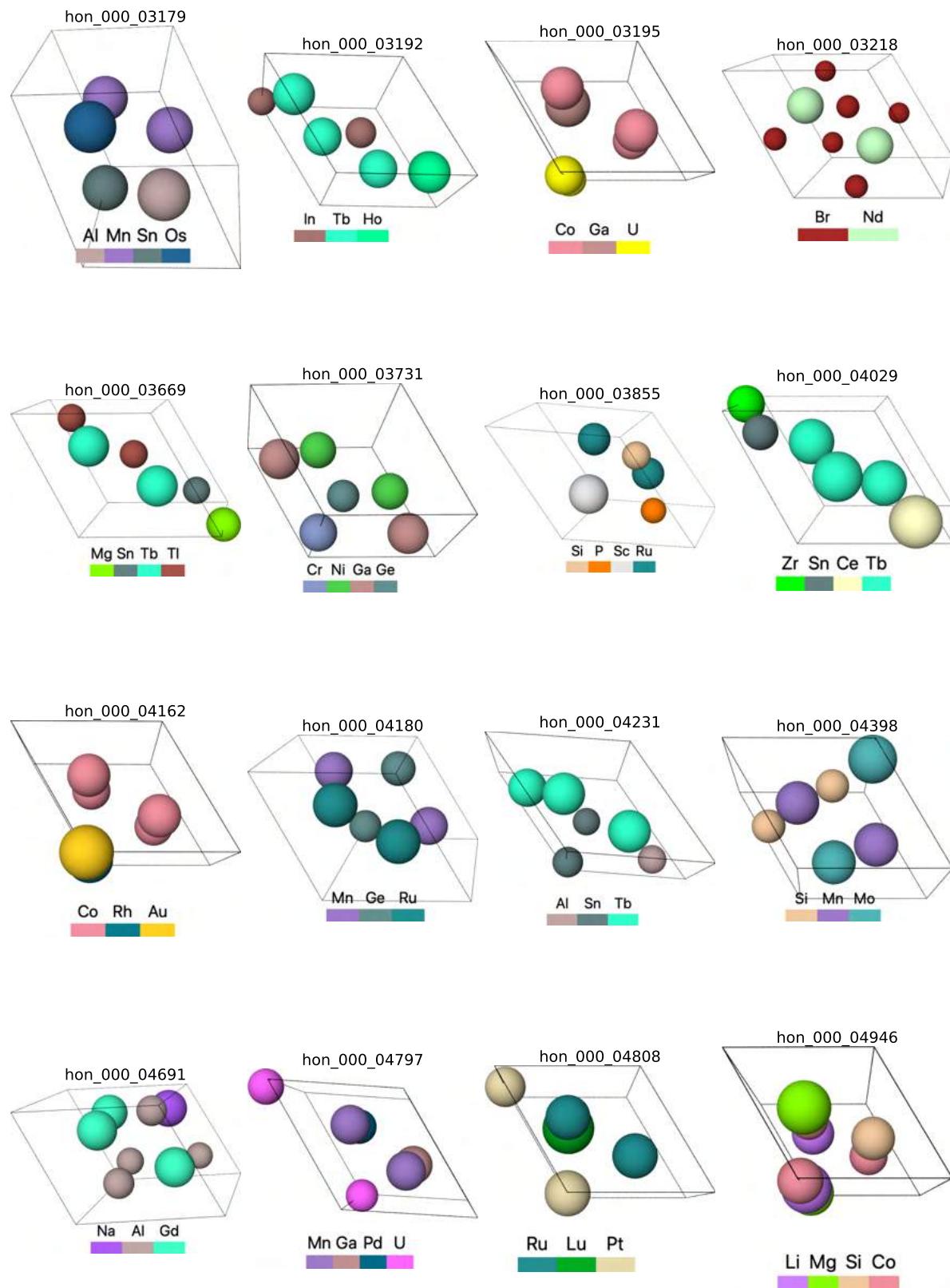


Figure S64. Generated materials with Honeycomb lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

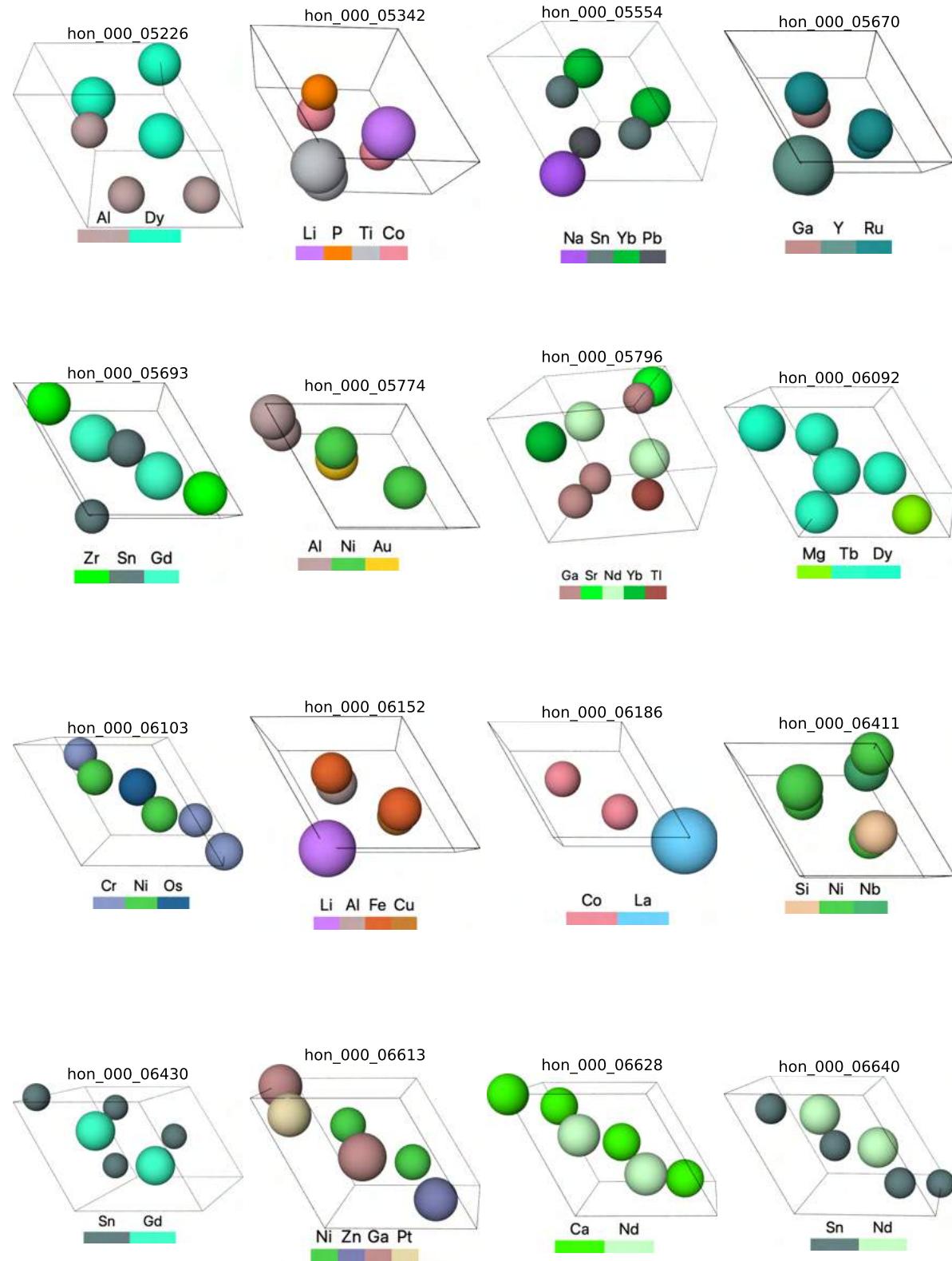


Figure S65. Generated materials with Honeycomb lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

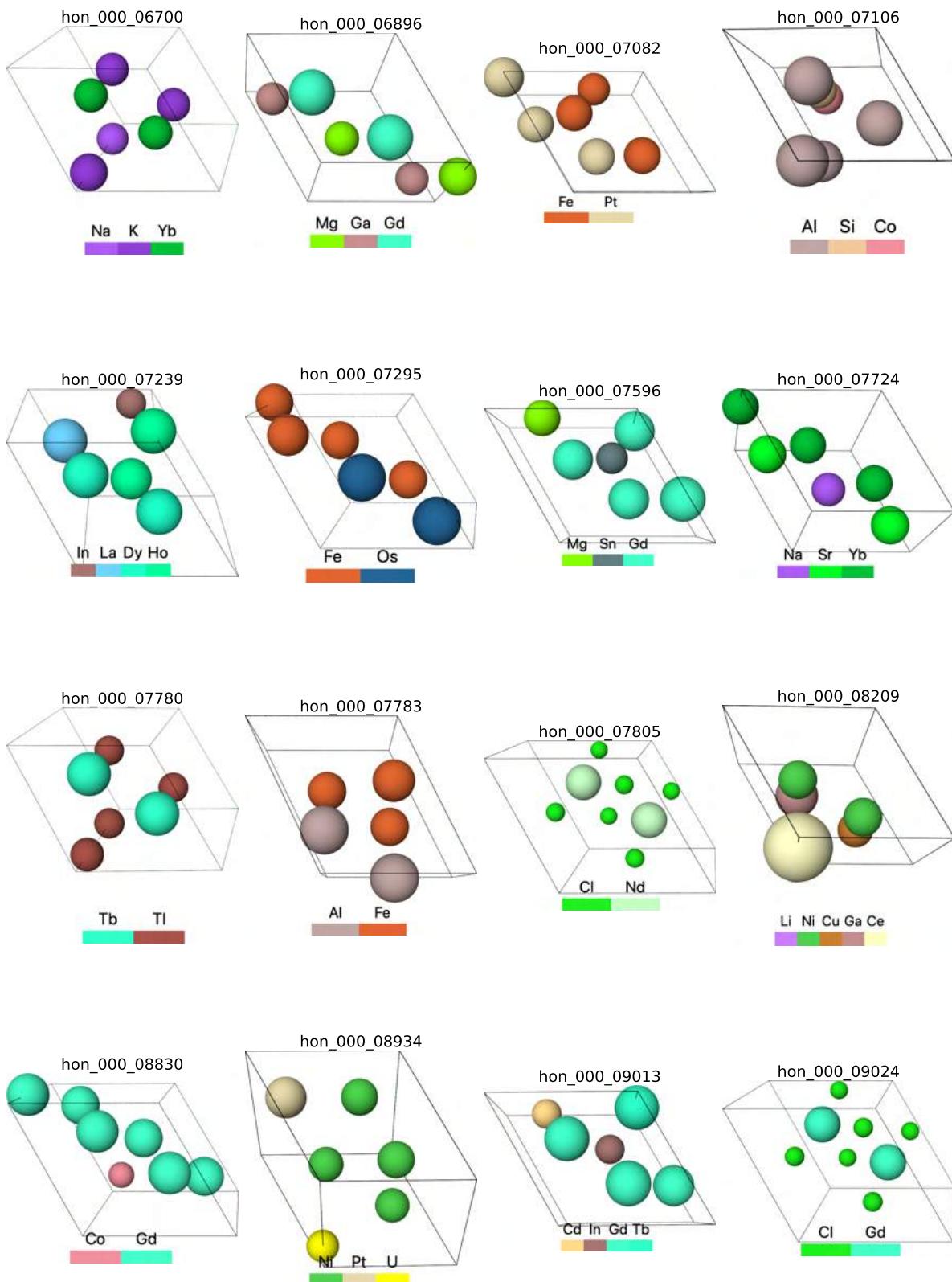


Figure S66. Generated materials with Honeycomb lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

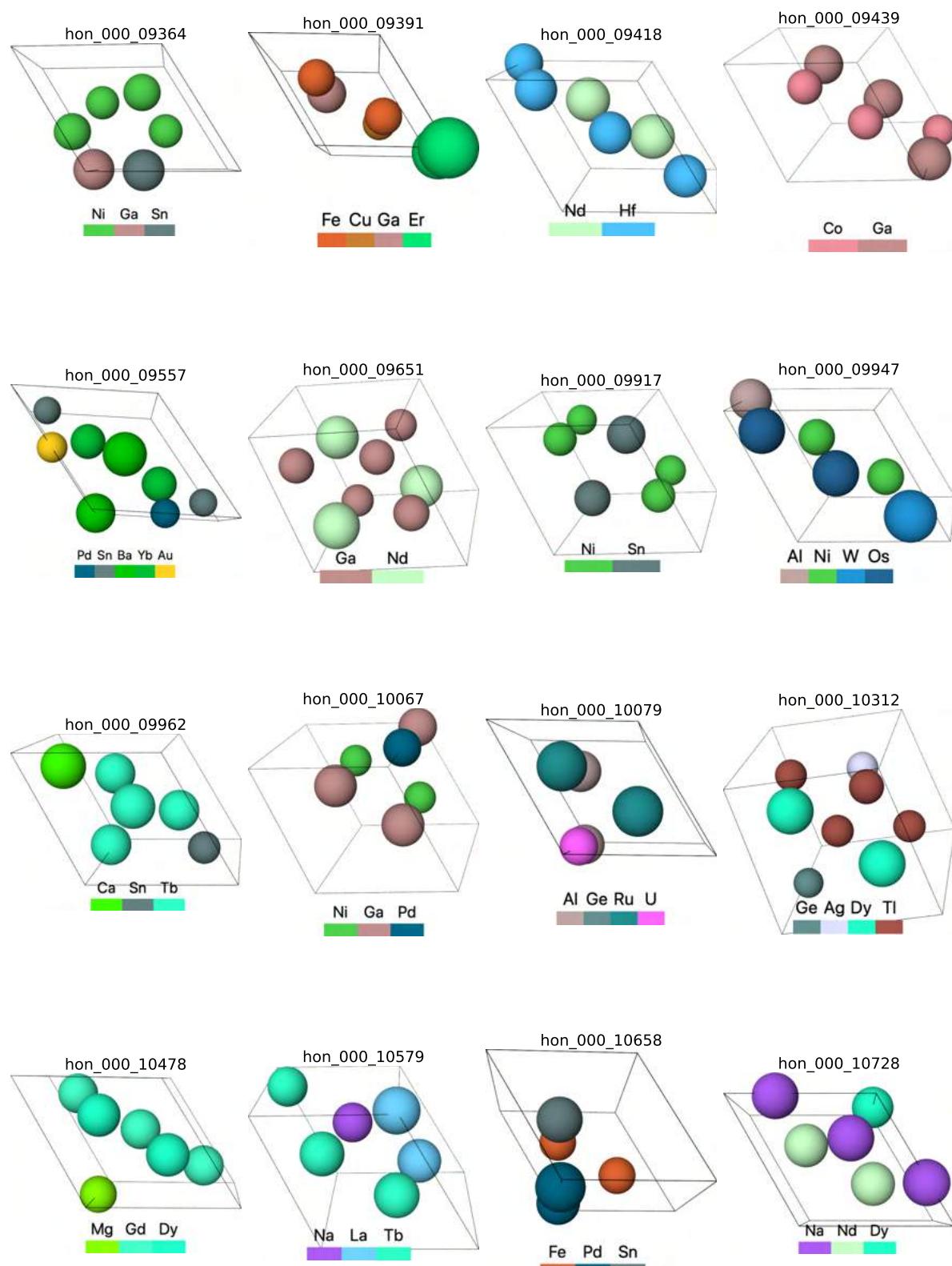


Figure S67. Generated materials with Honeycomb lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

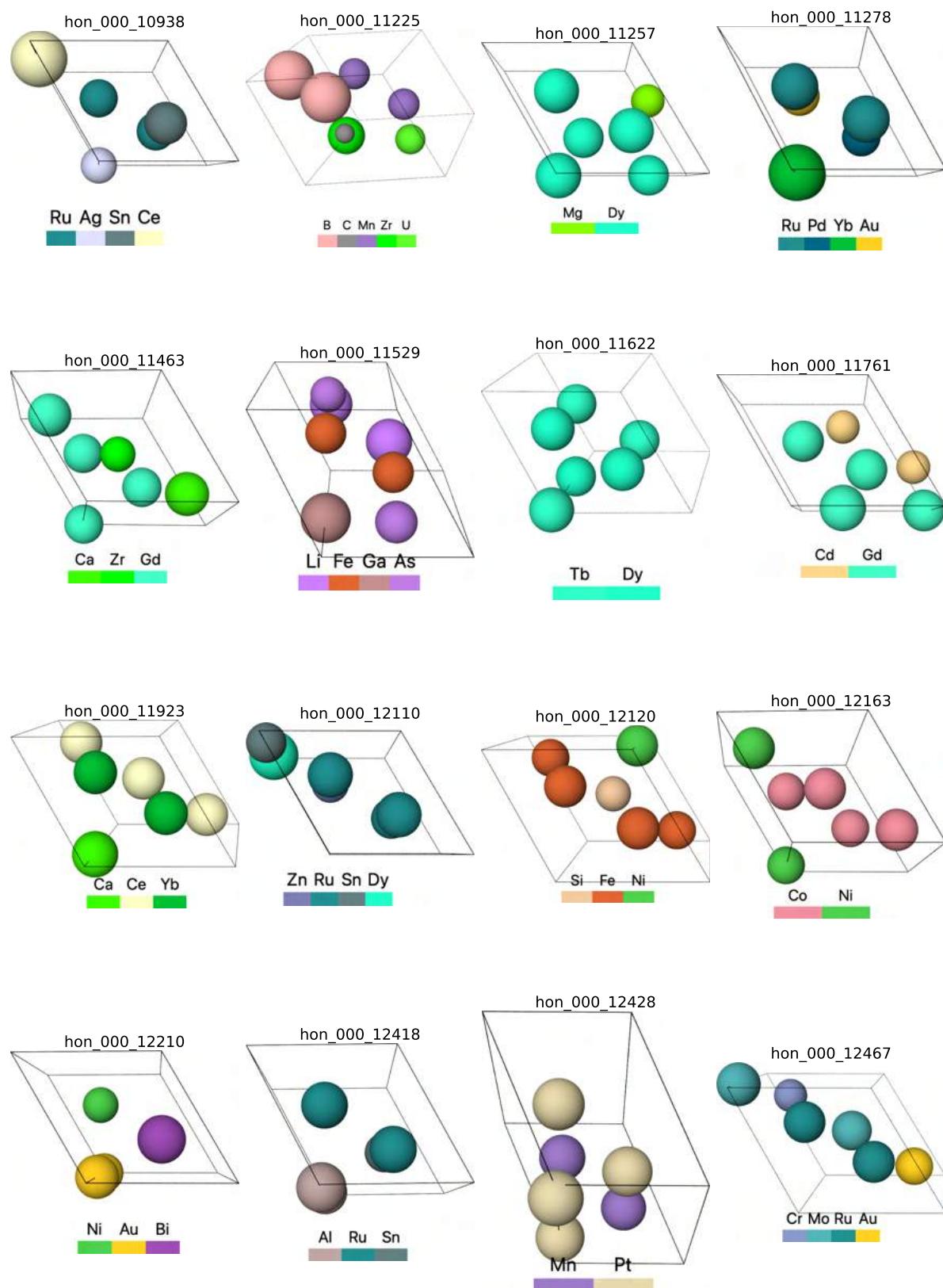


Figure S68. Generated materials with Honeycomb lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

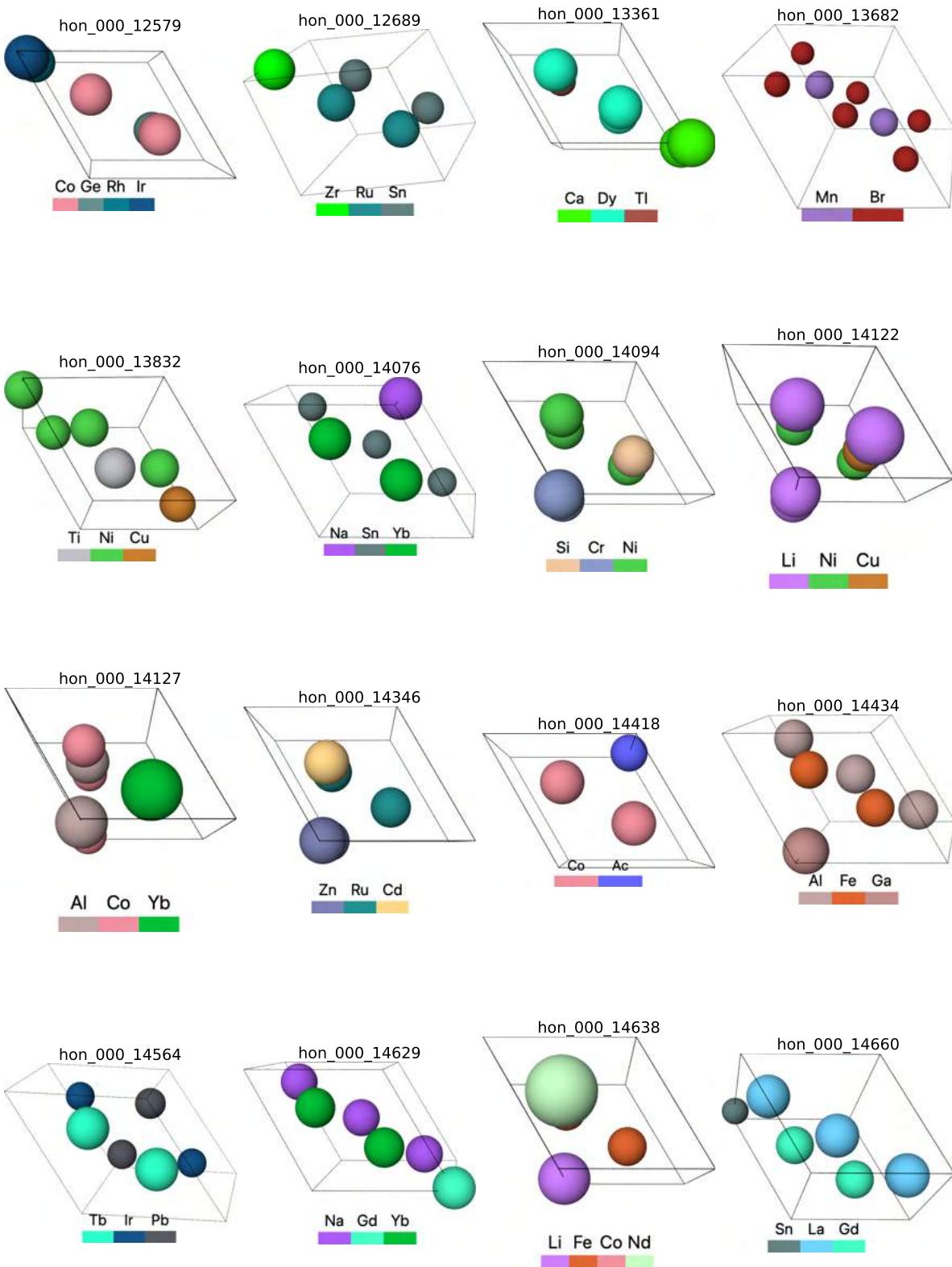


Figure S69. Generated materials with Honeycomb lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

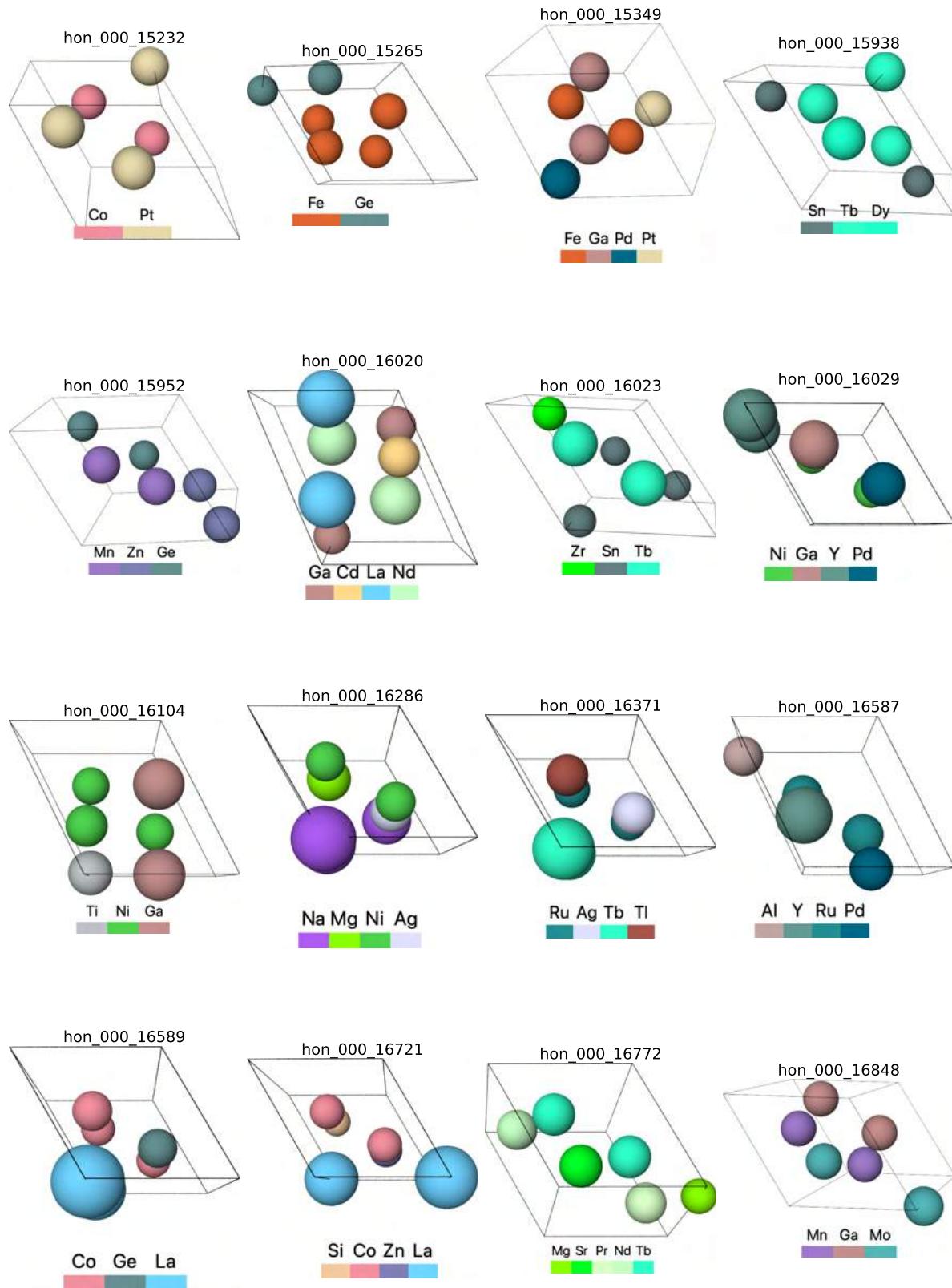


Figure S70. Generated materials with Honeycomb lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

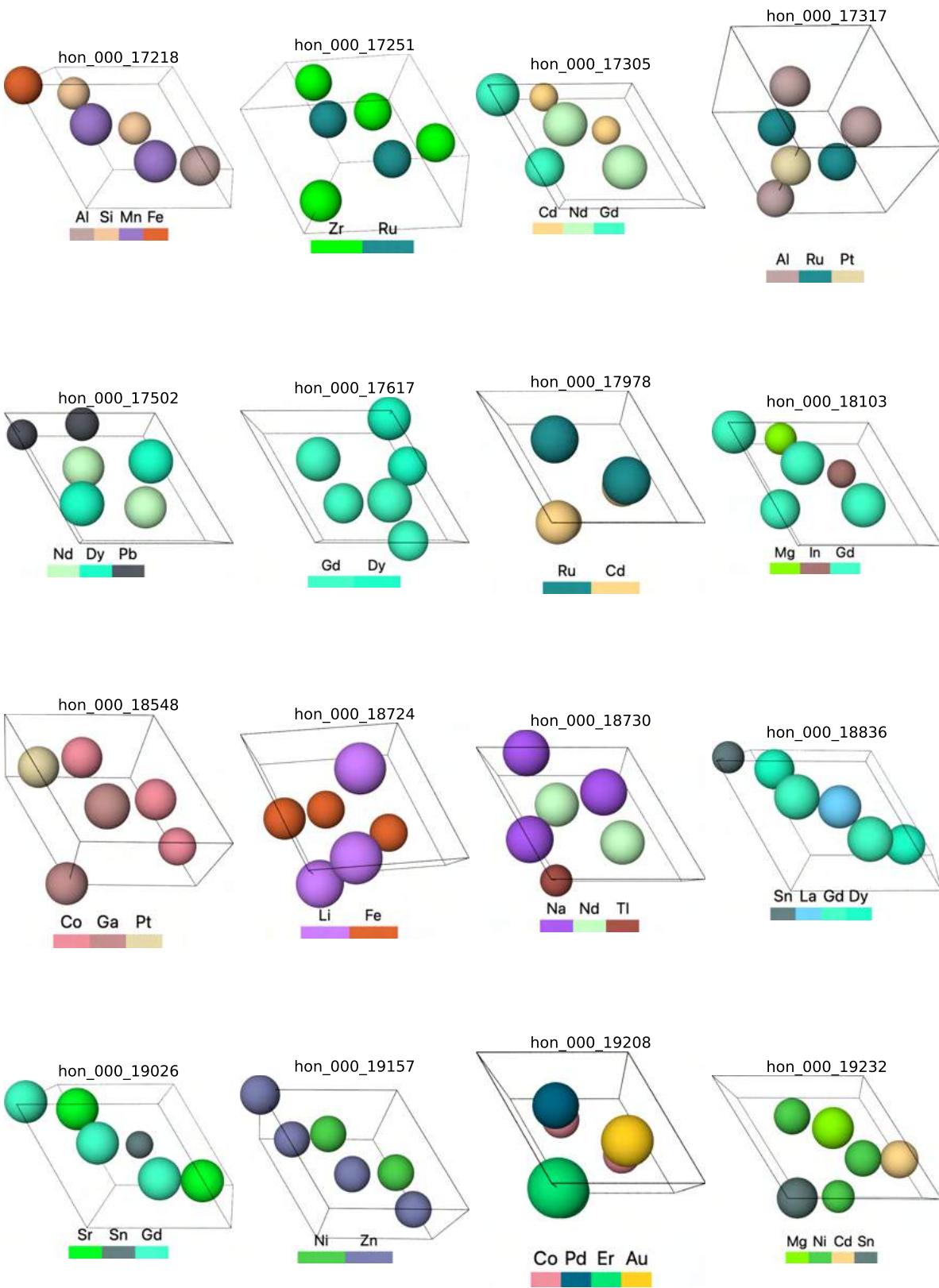


Figure S71. Generated materials with Honeycomb lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

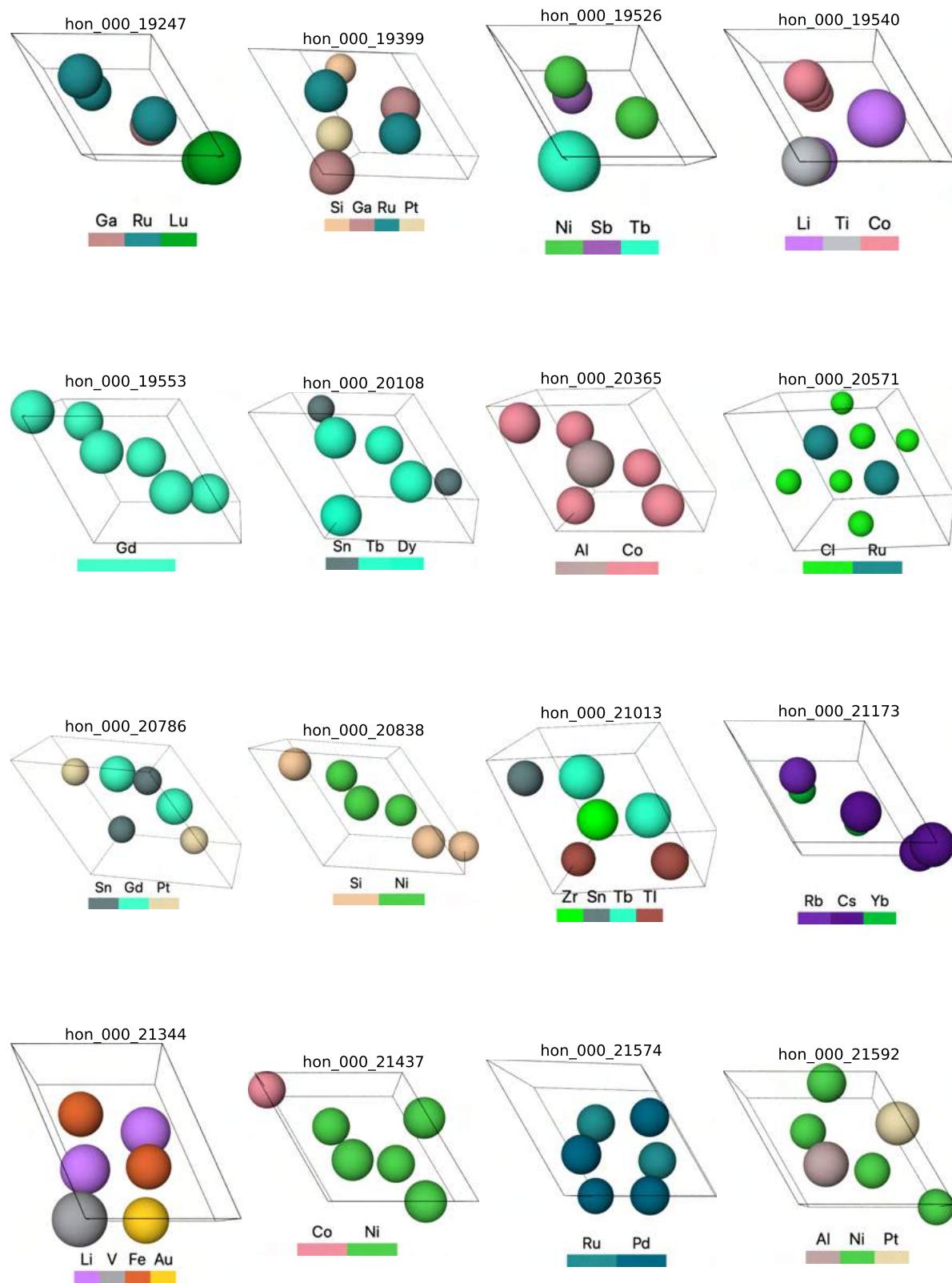


Figure S72. Generated materials with Honeycomb lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

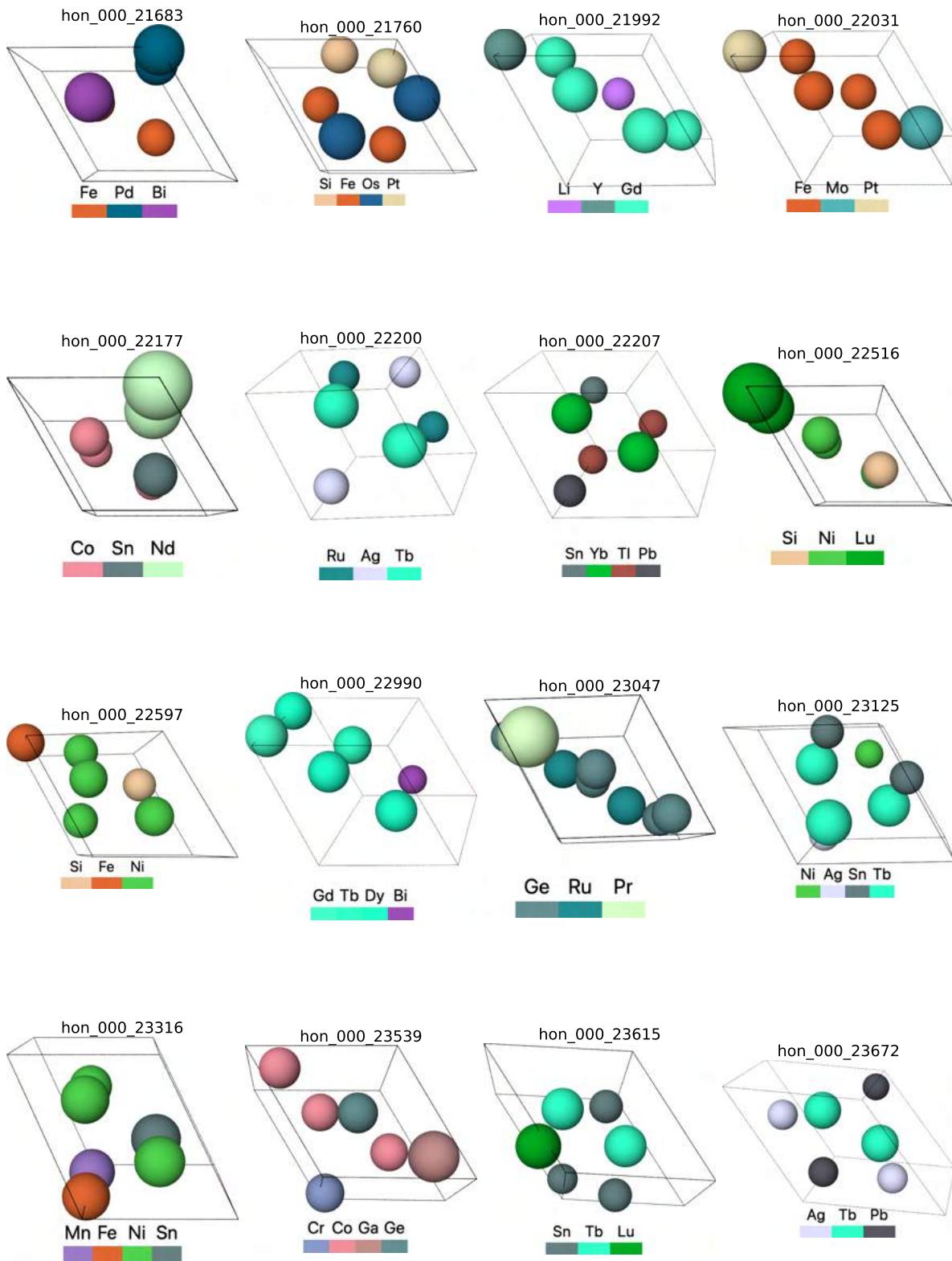


Figure S73. Generated materials with Honeycomb lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

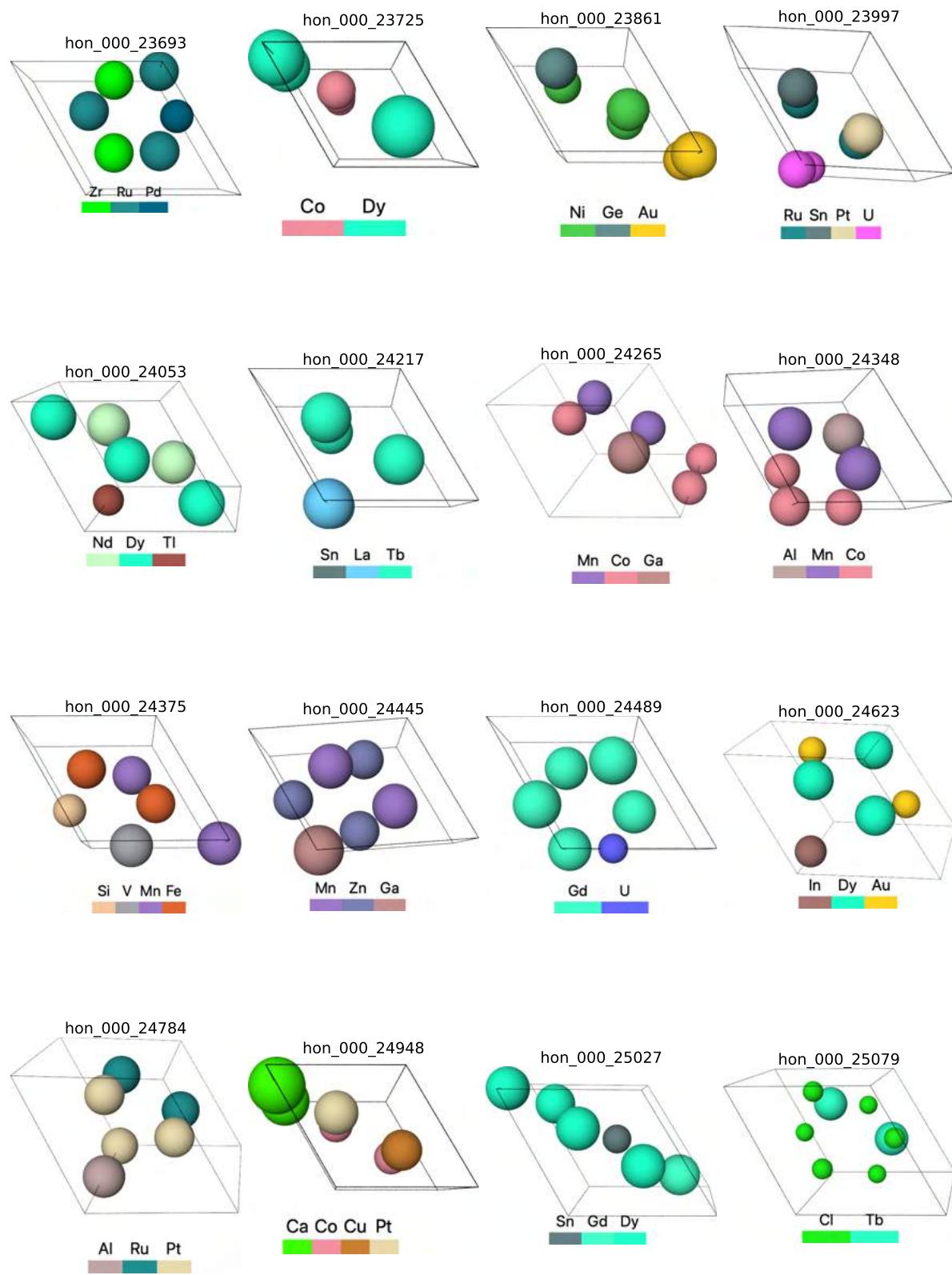


Figure S74. Generated materials with Honeycomb lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

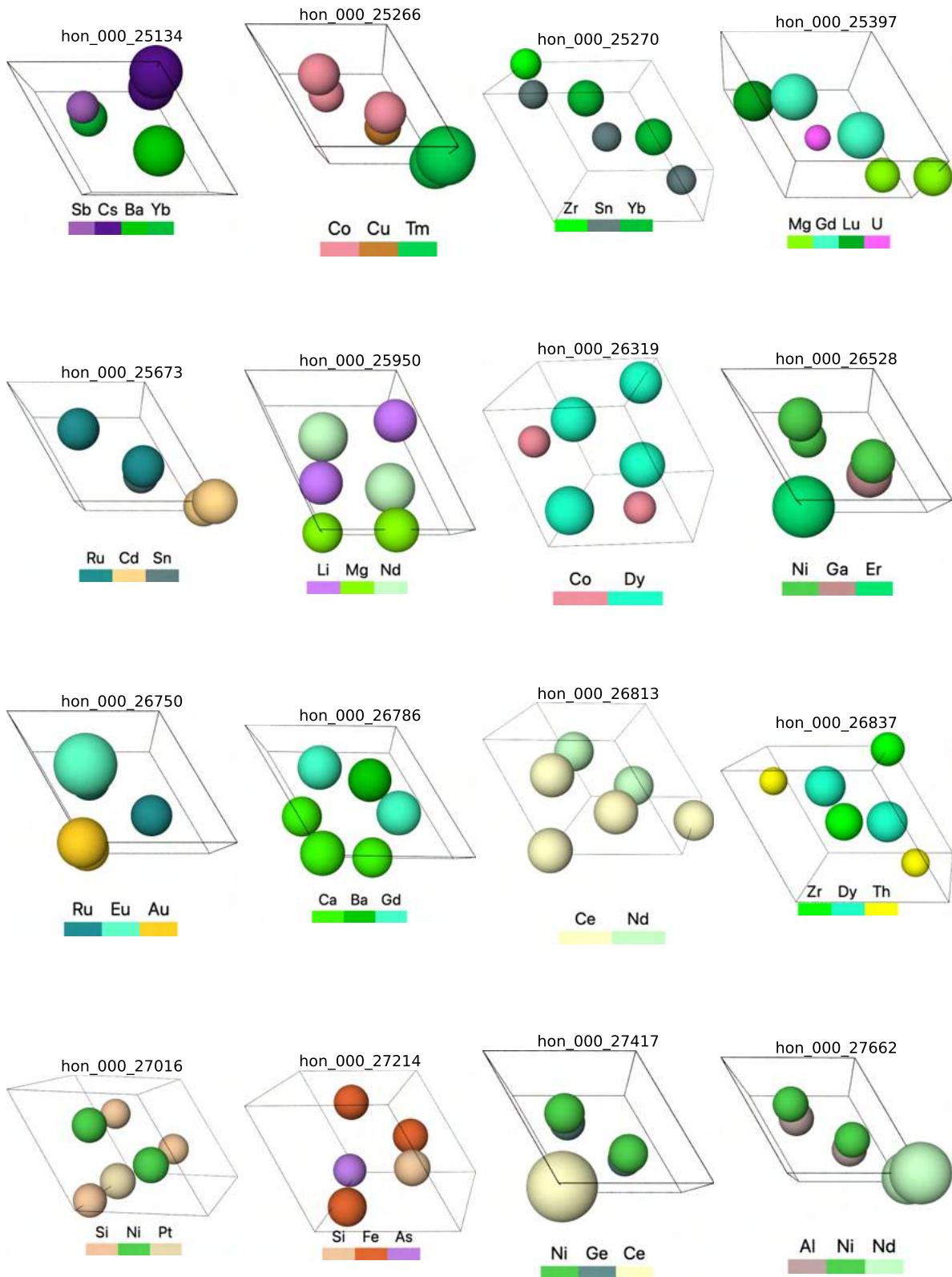


Figure S75. Generated materials with Honeycomb lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

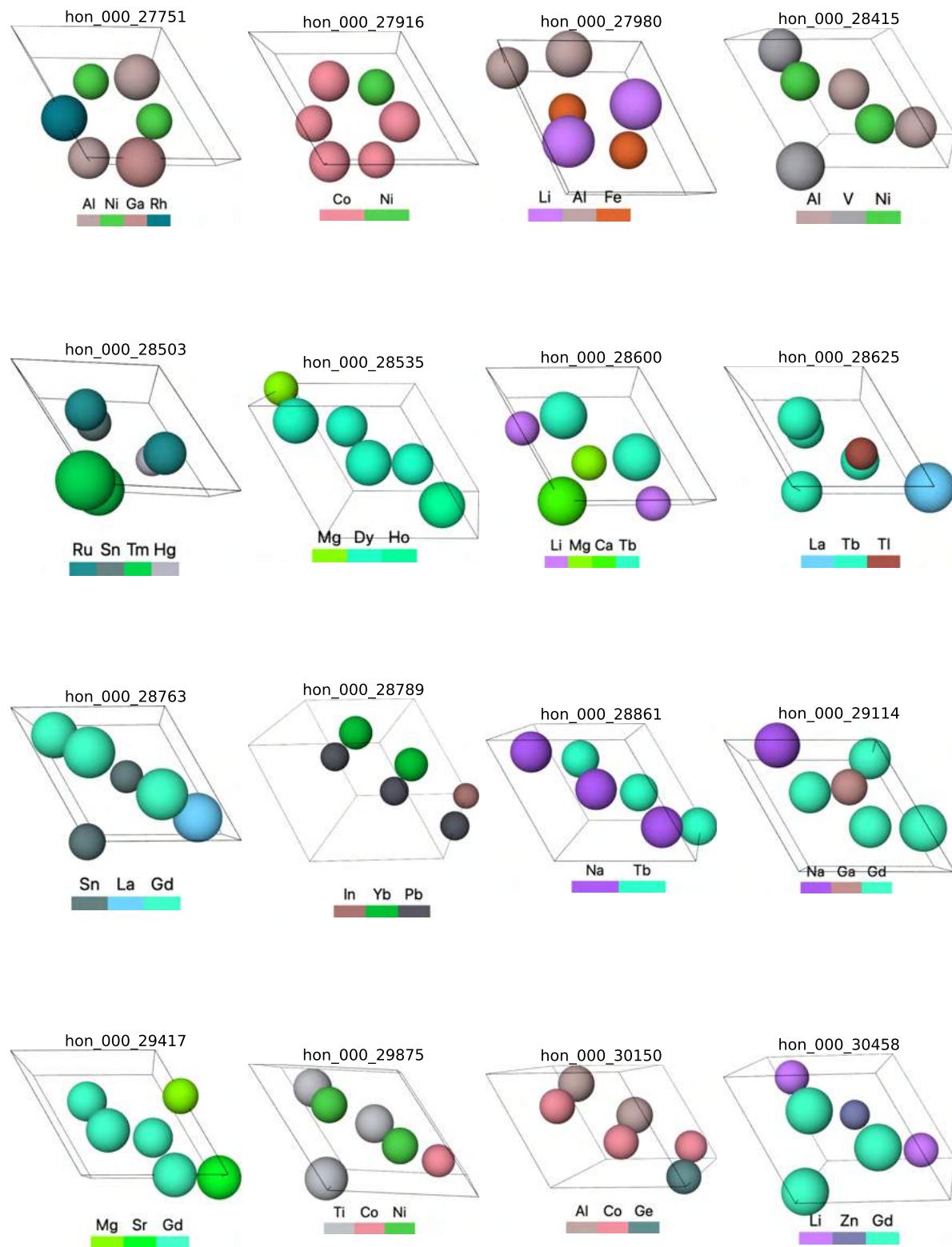


Figure S76. Generated materials with Honeycomb lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

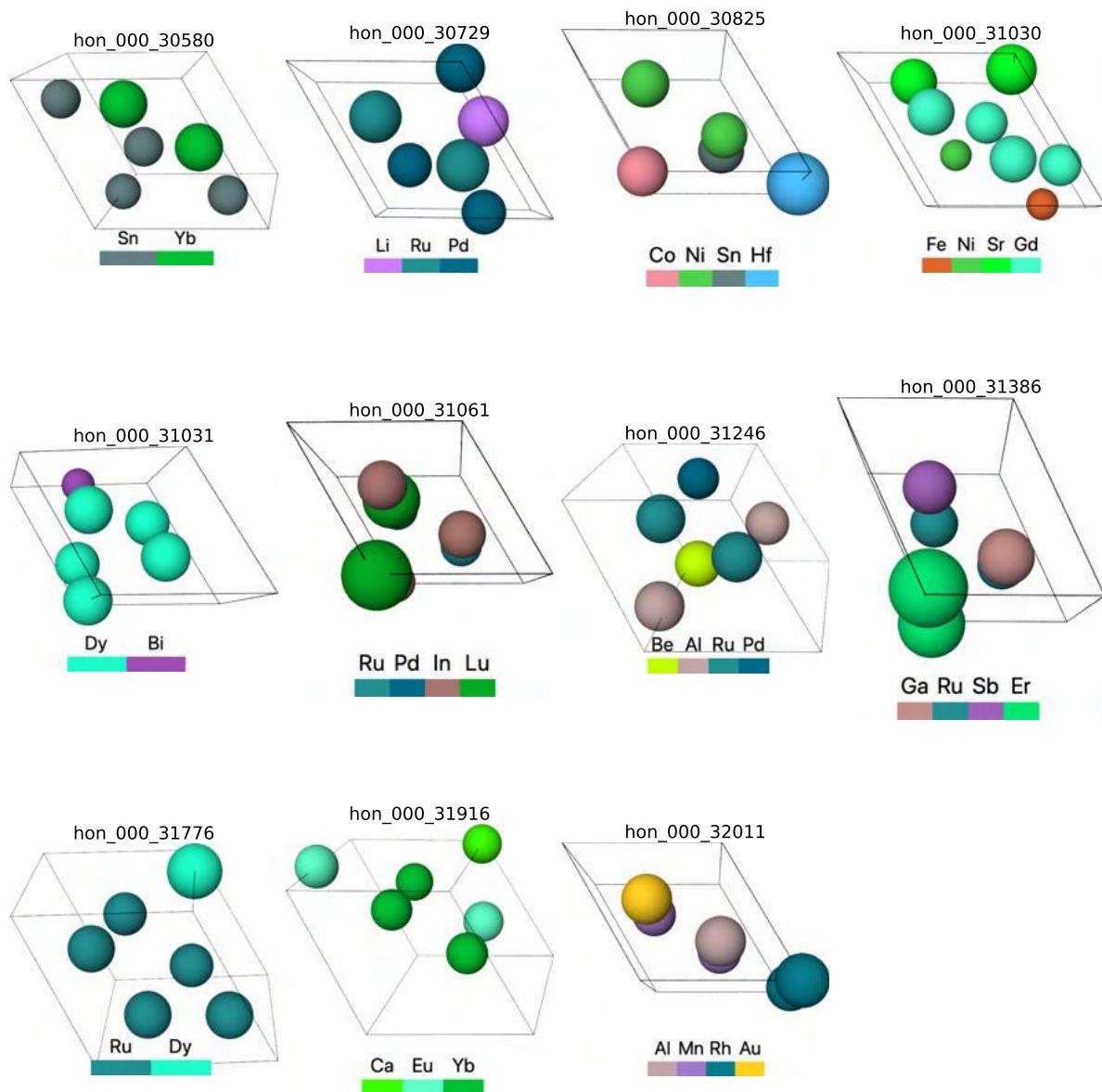


Figure S77. Generated materials with Honeycomb lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

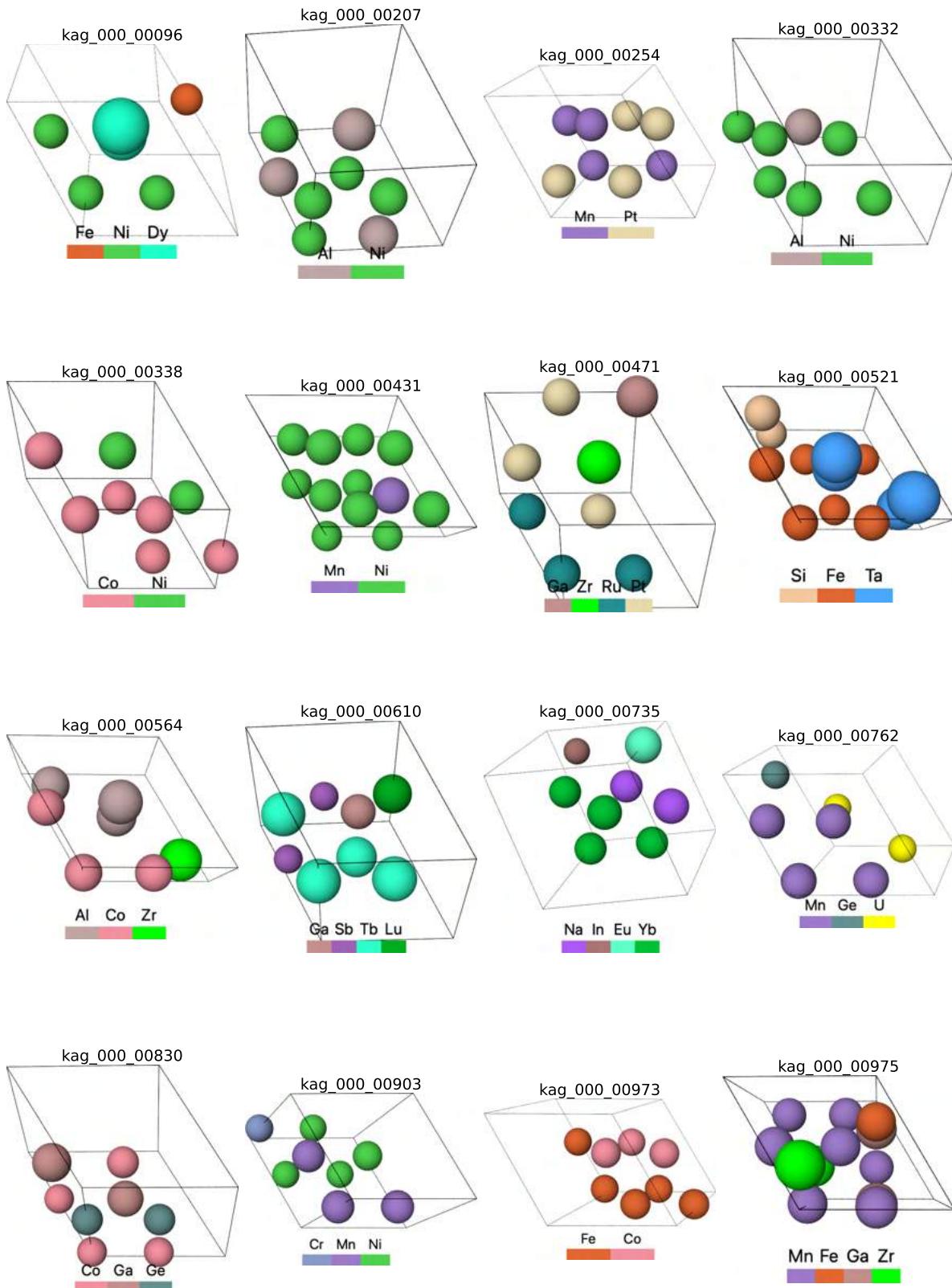


Figure S78. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

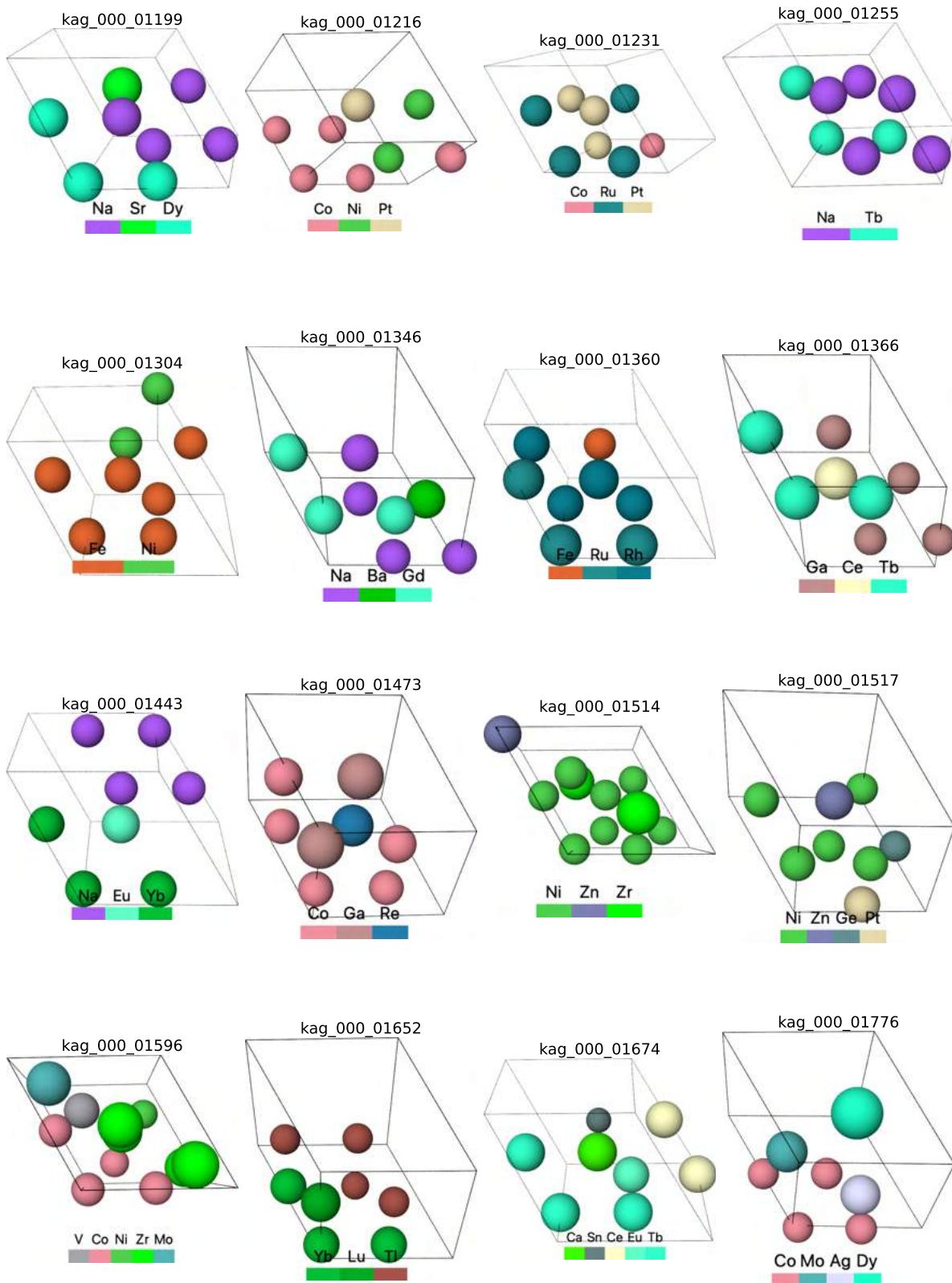


Figure S79. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

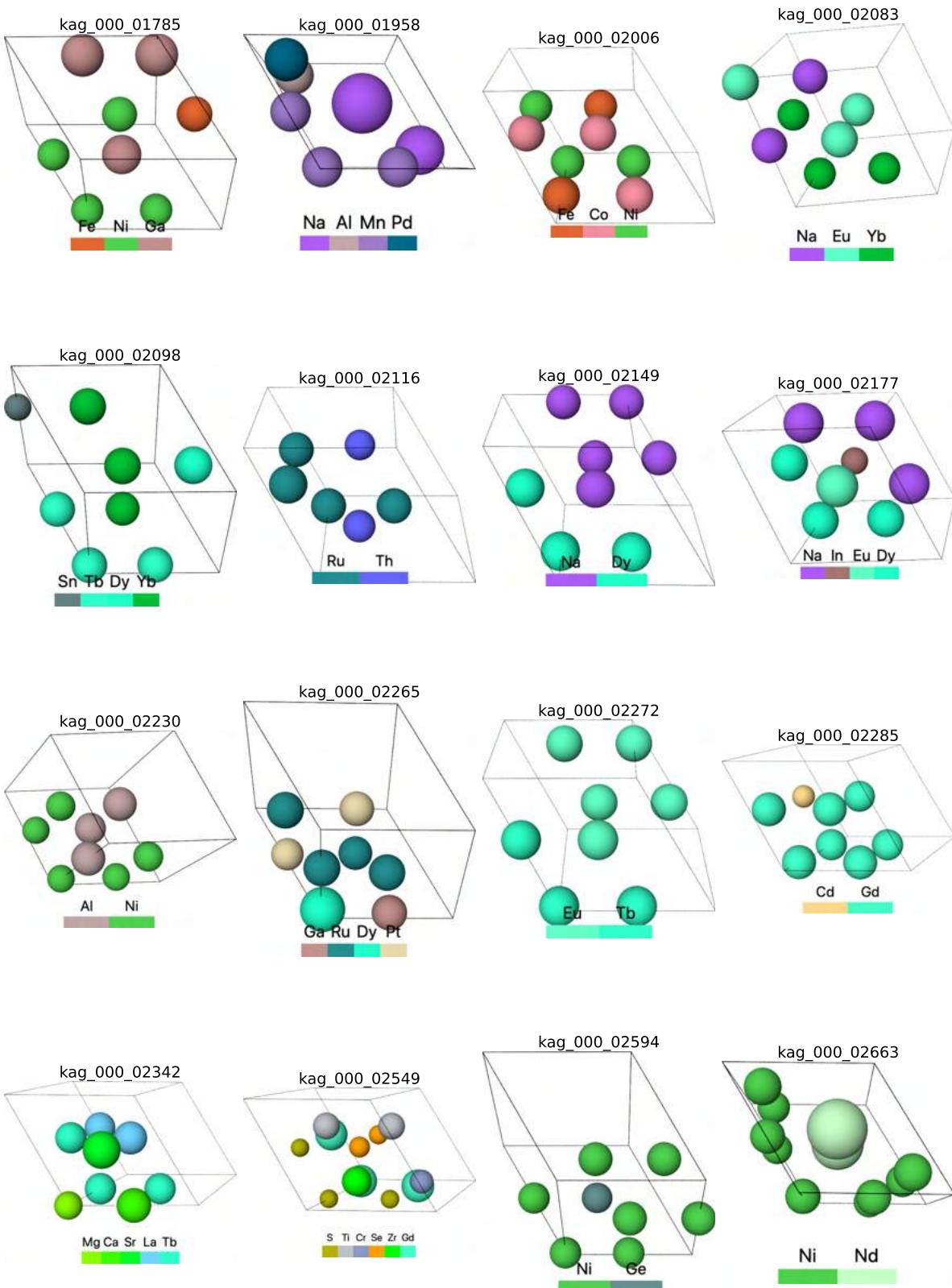


Figure S80. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

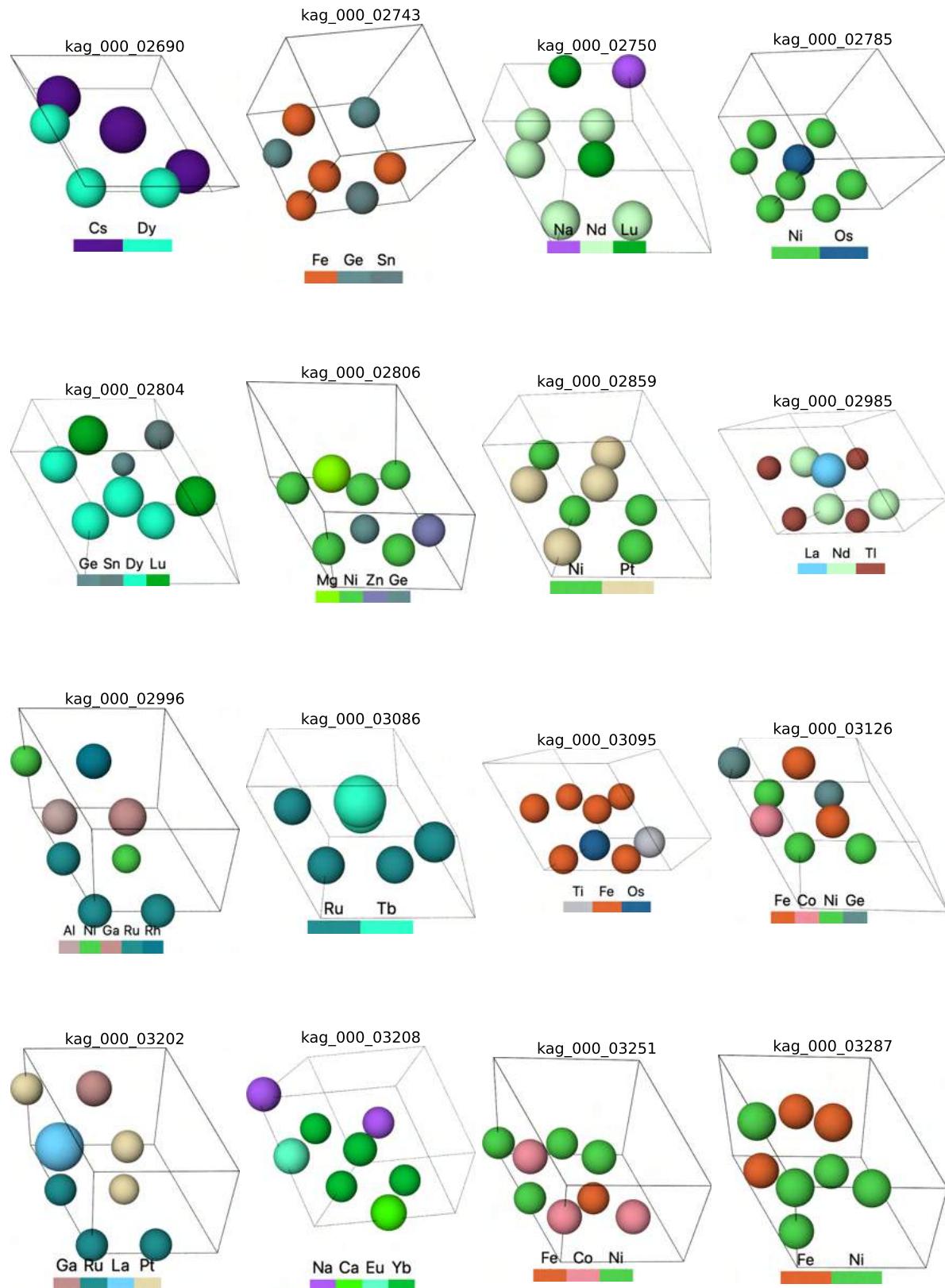


Figure S81. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

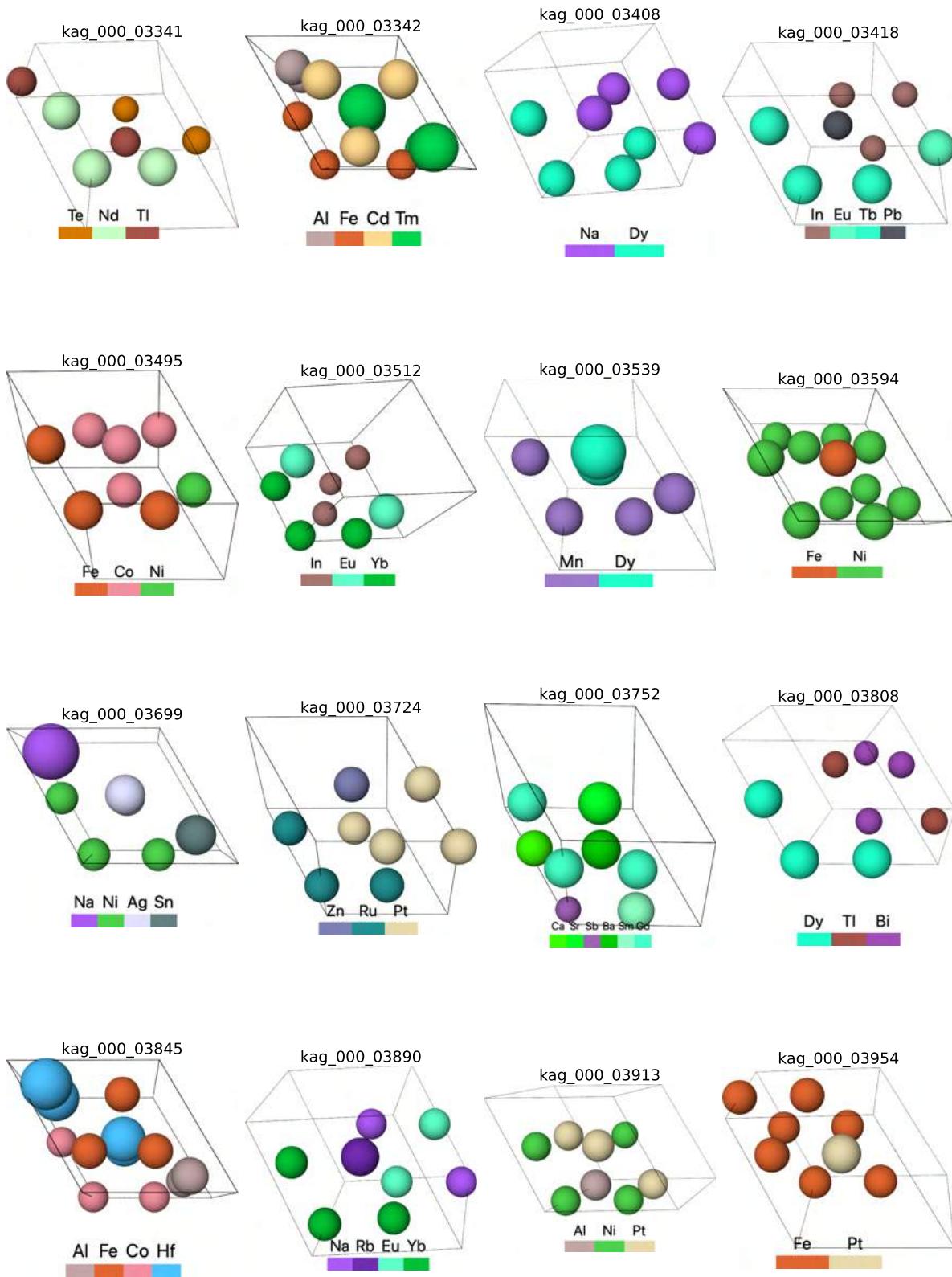


Figure S82. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

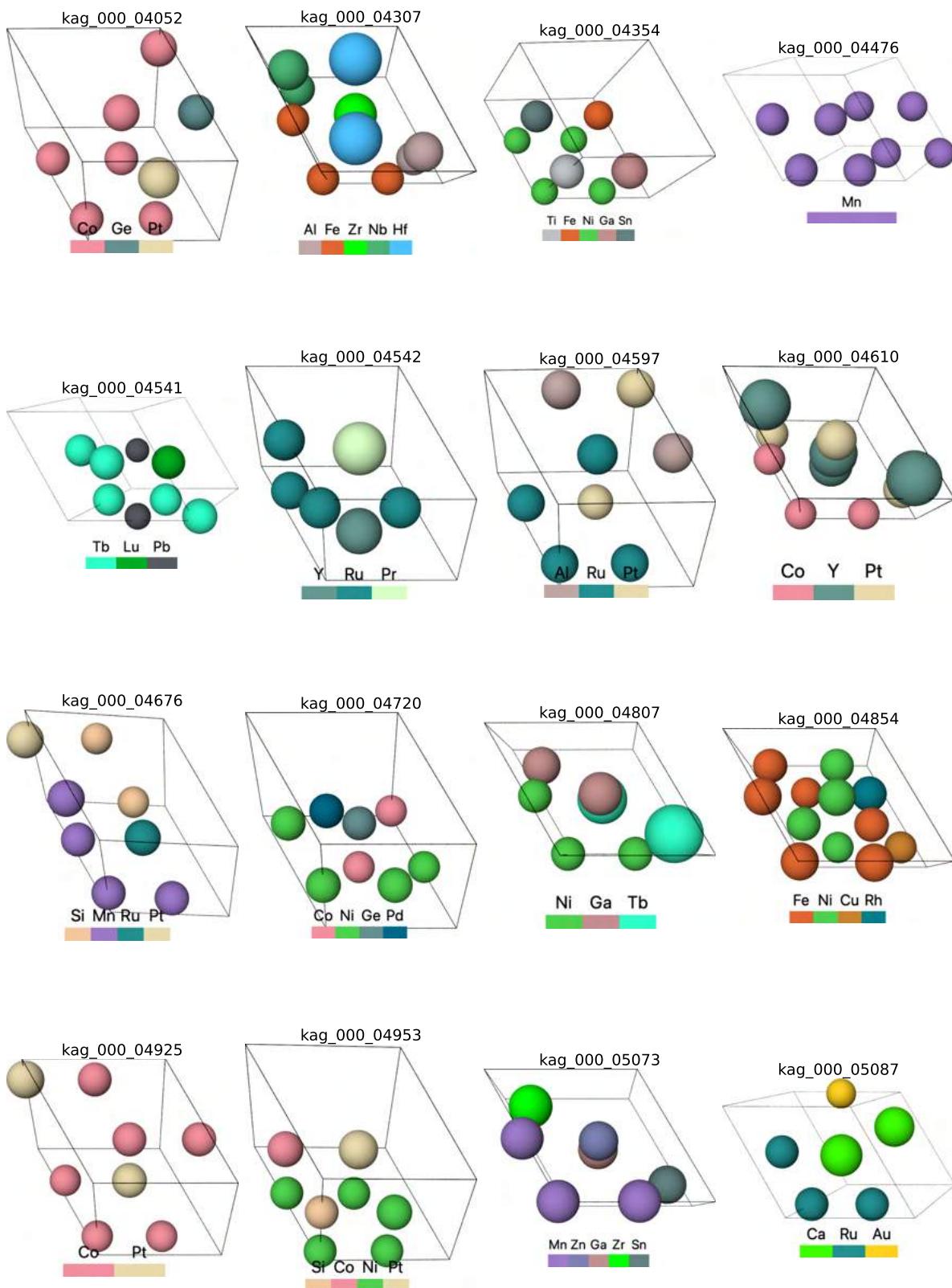


Figure S83. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

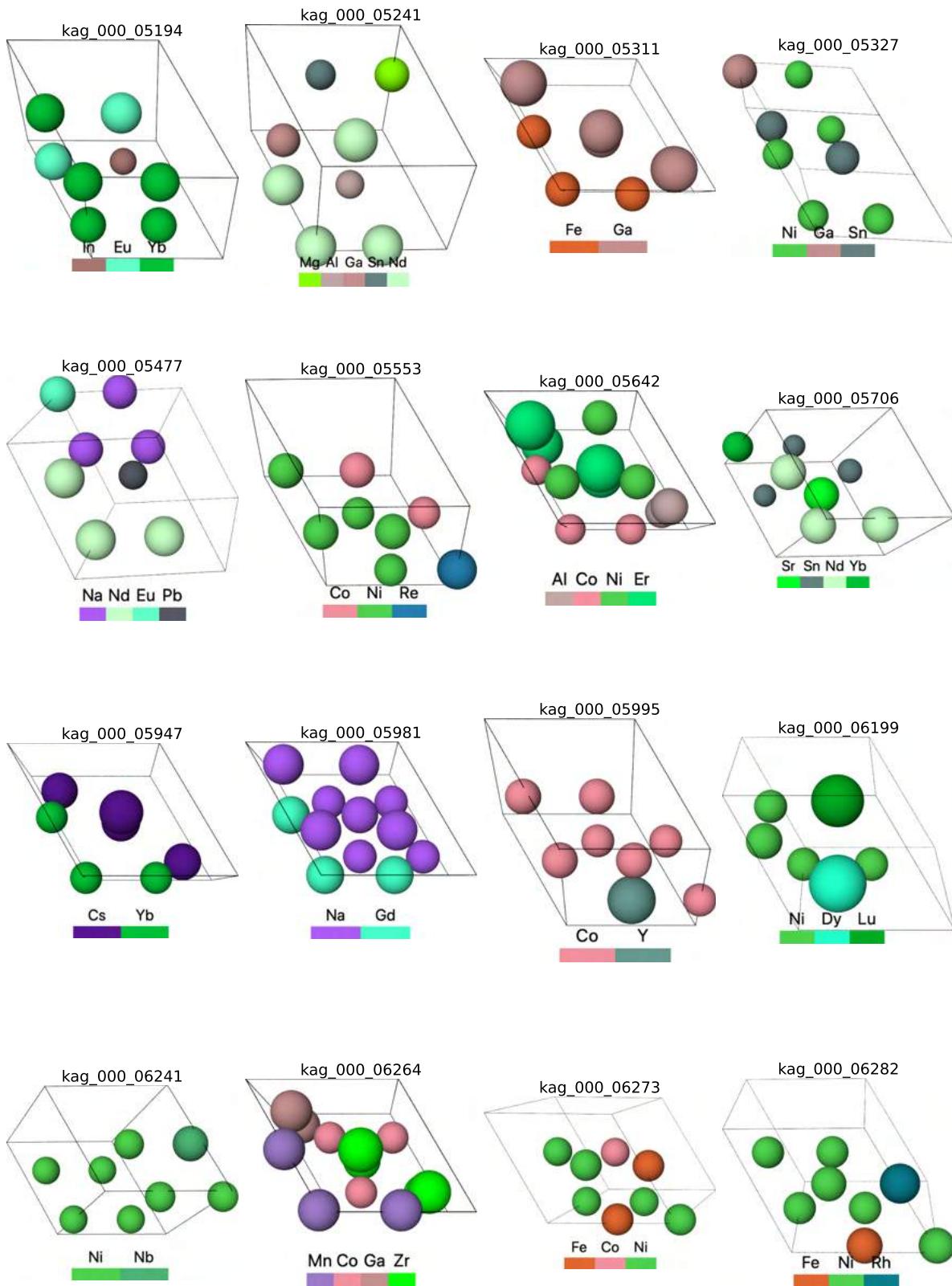


Figure S84. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

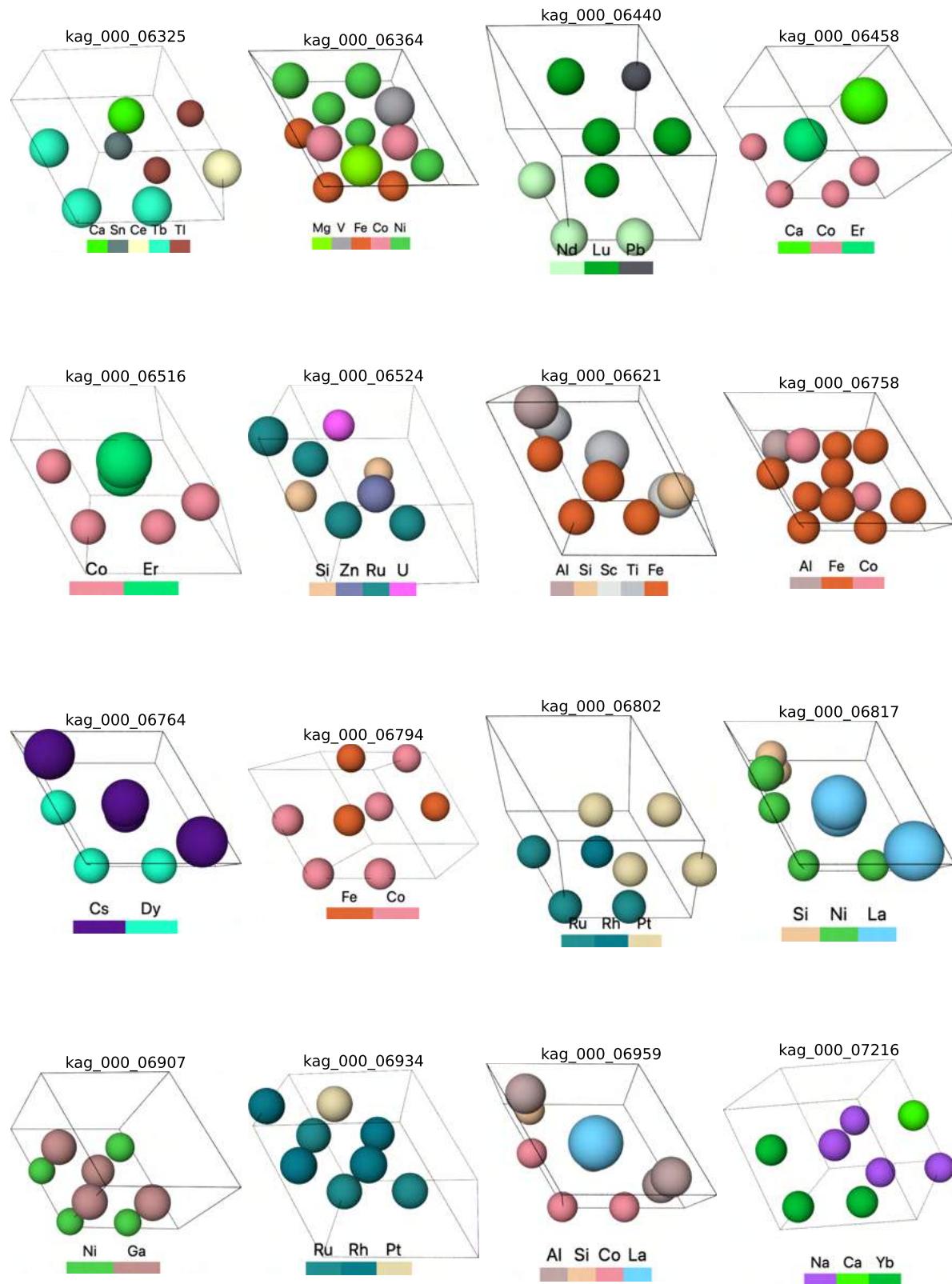


Figure S85. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

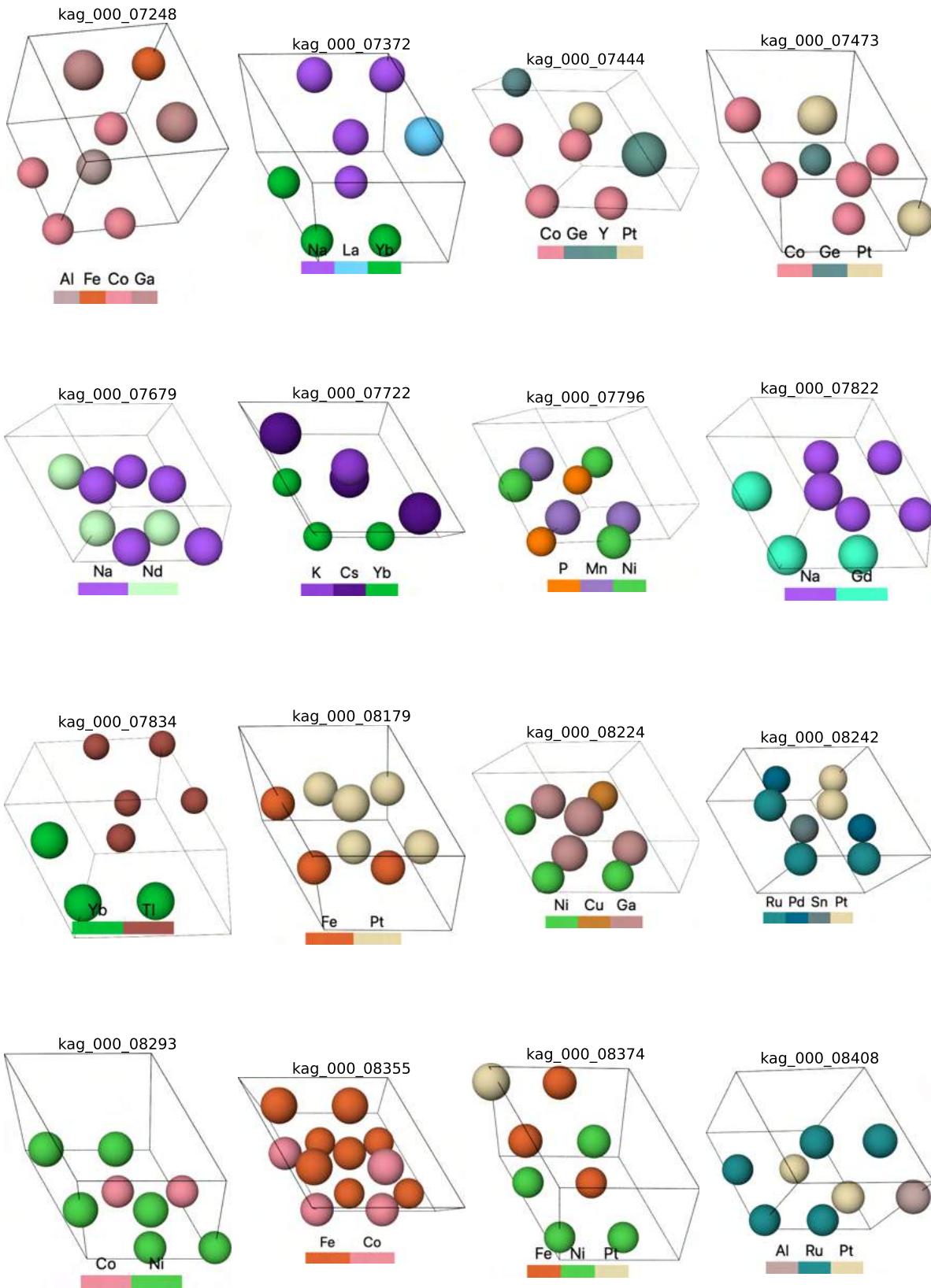


Figure S86. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

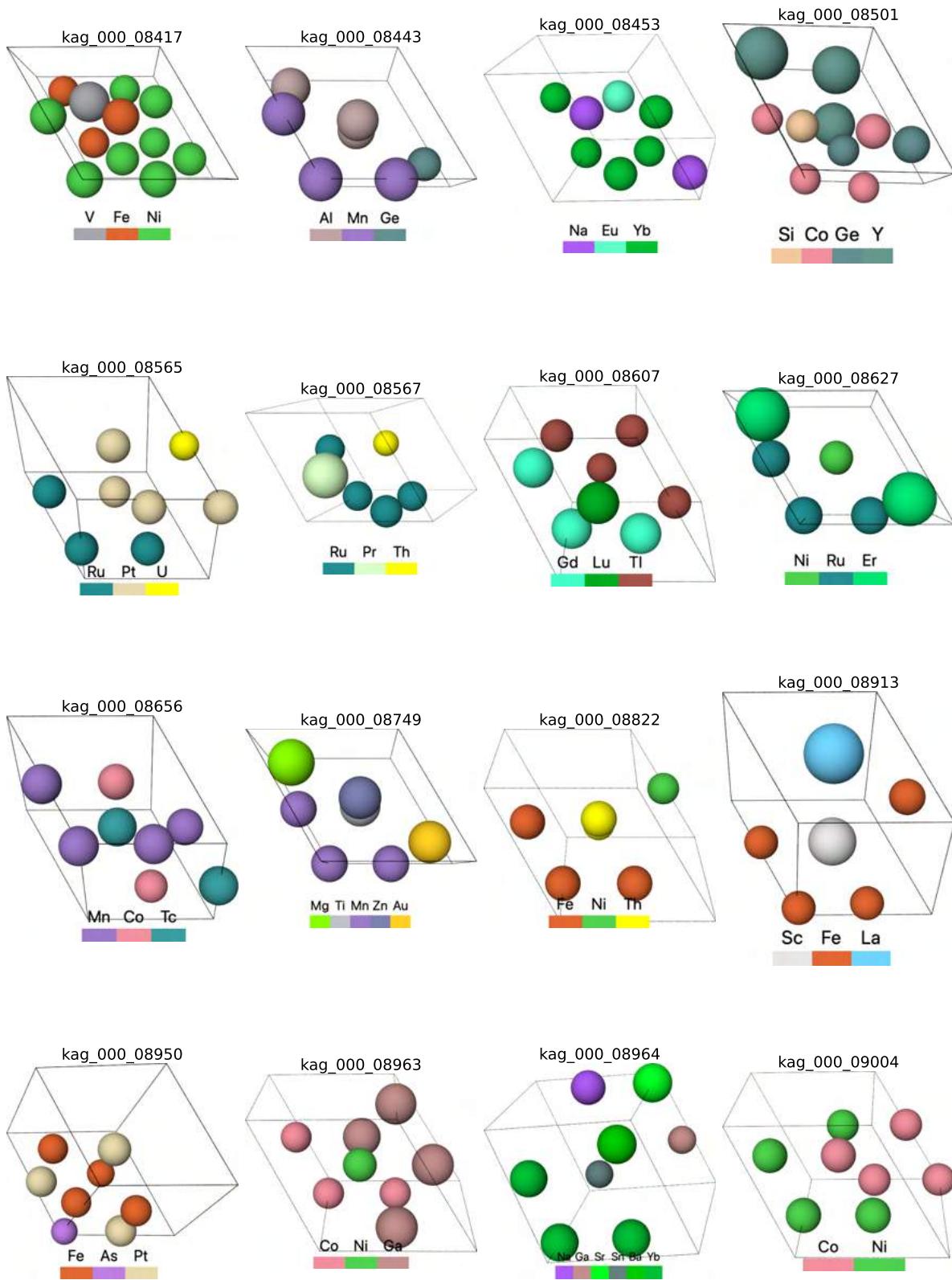


Figure S87. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

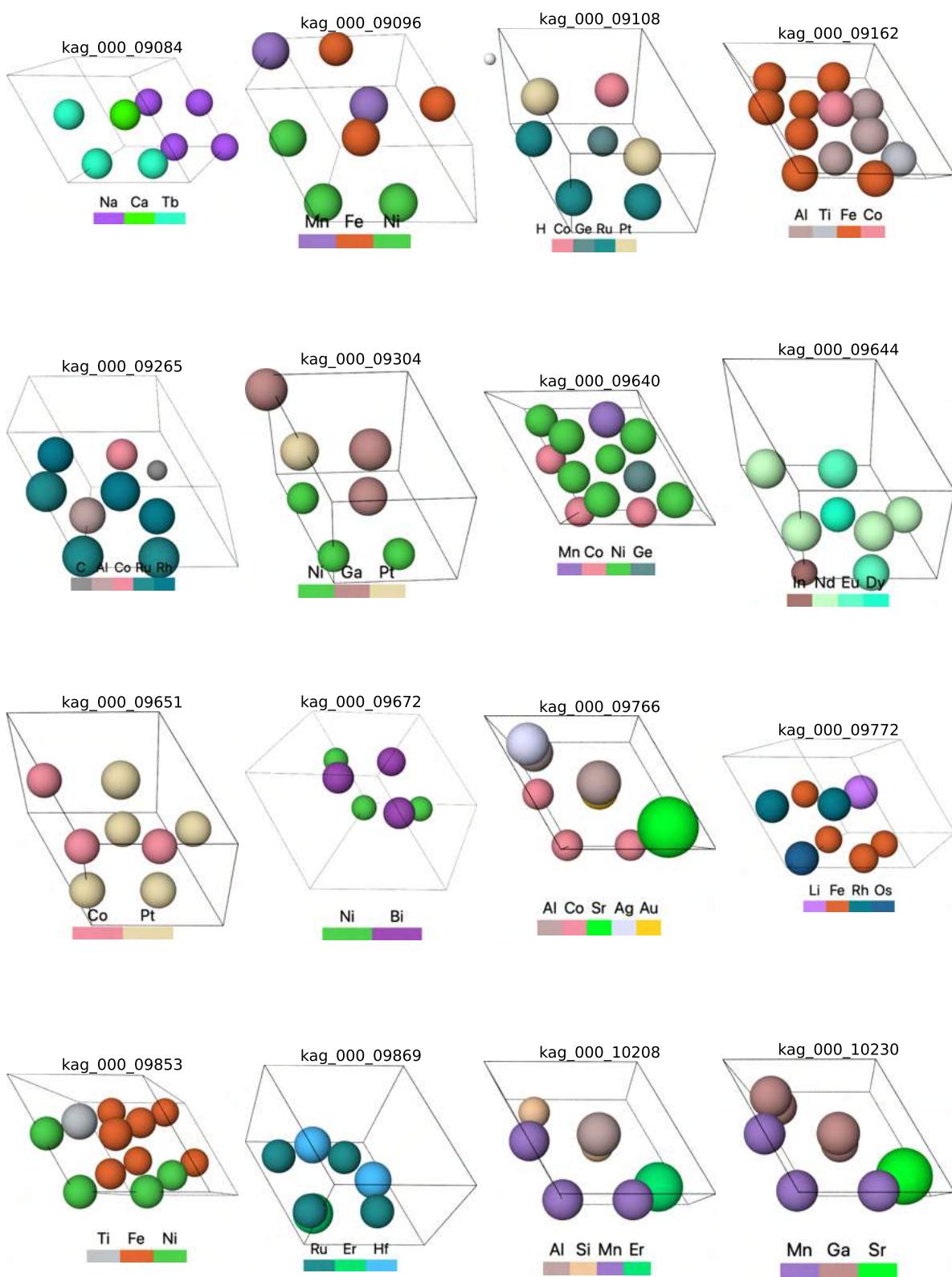


Figure S88. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

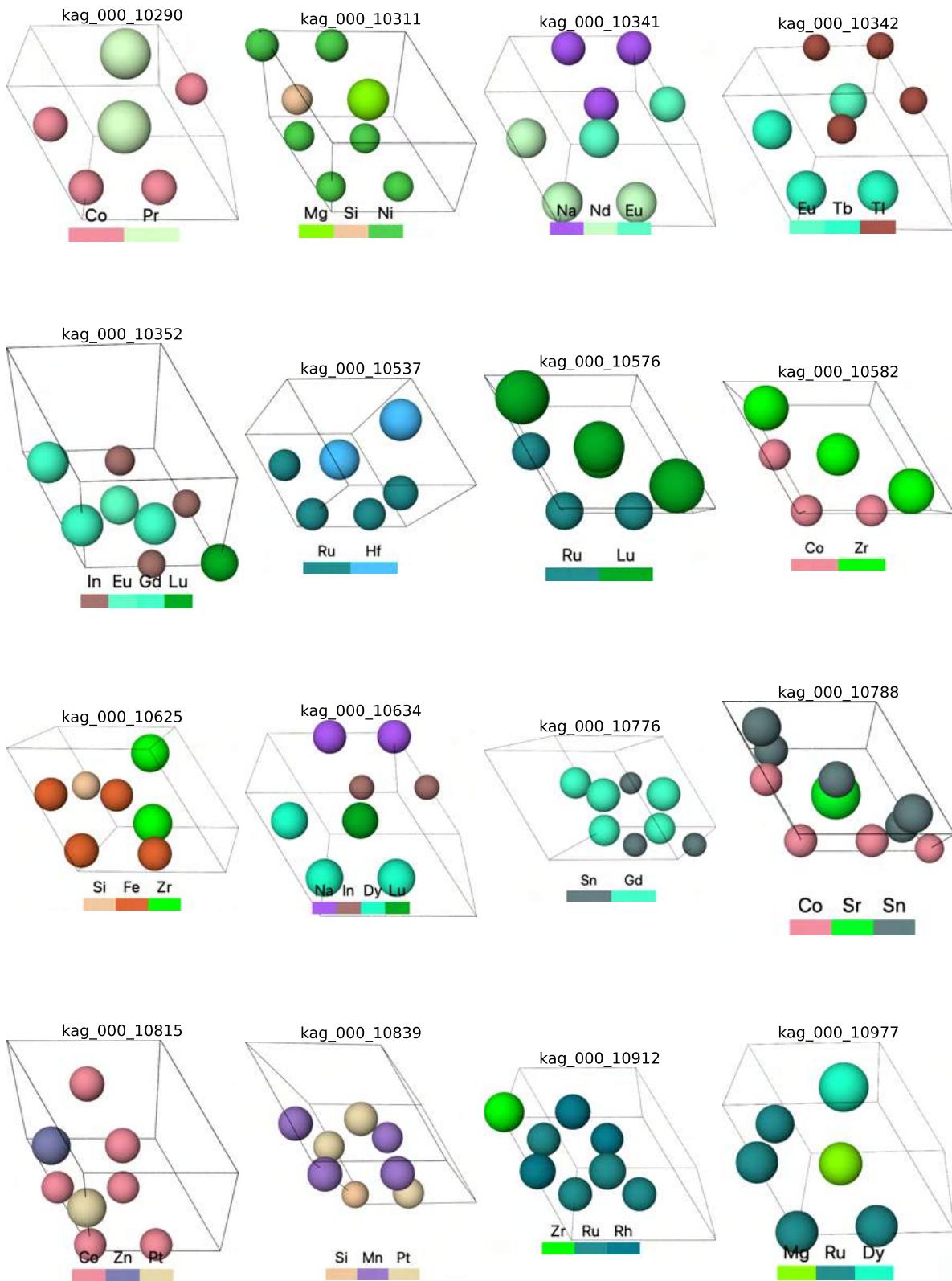


Figure S89. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

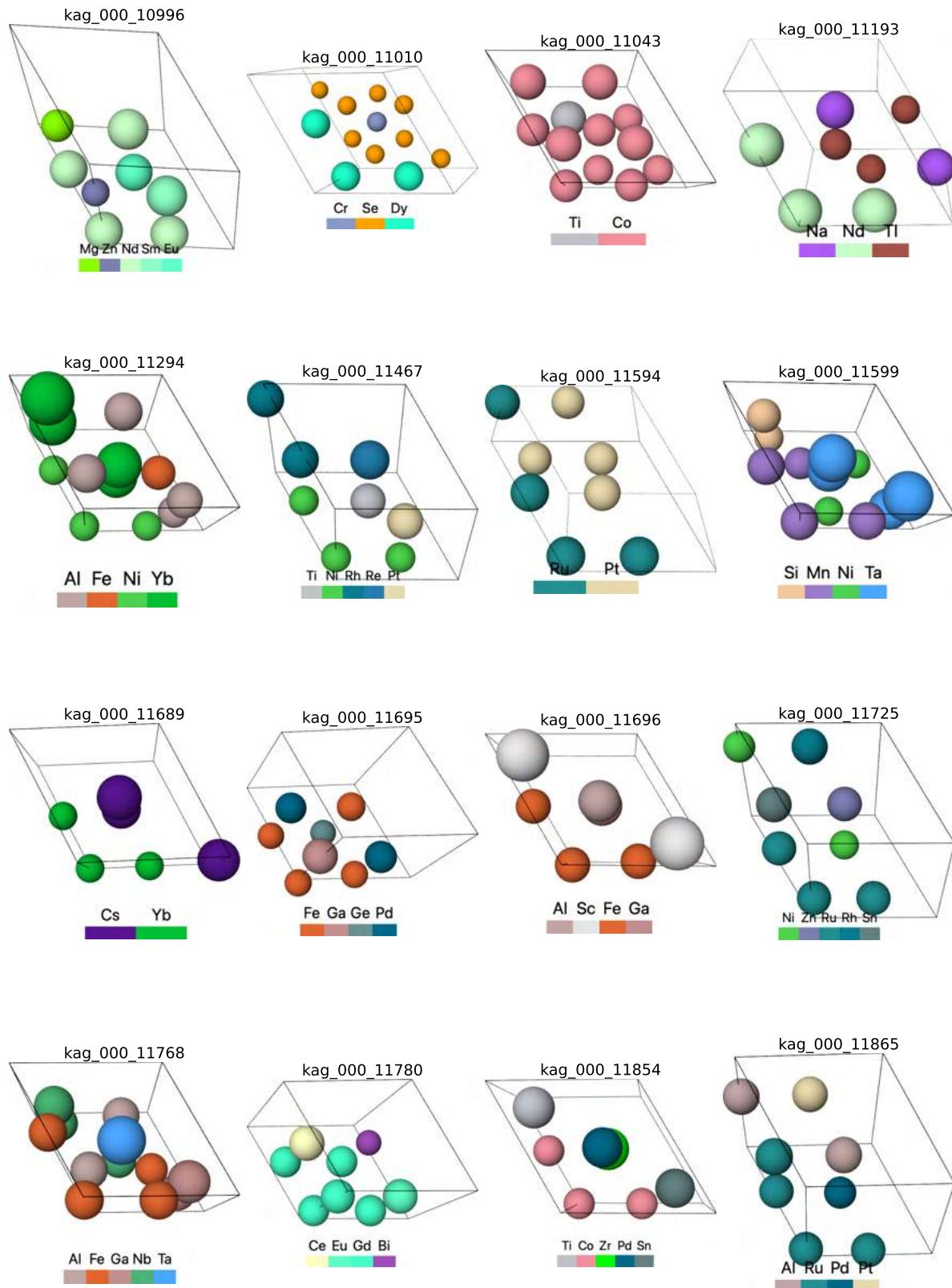


Figure S90. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

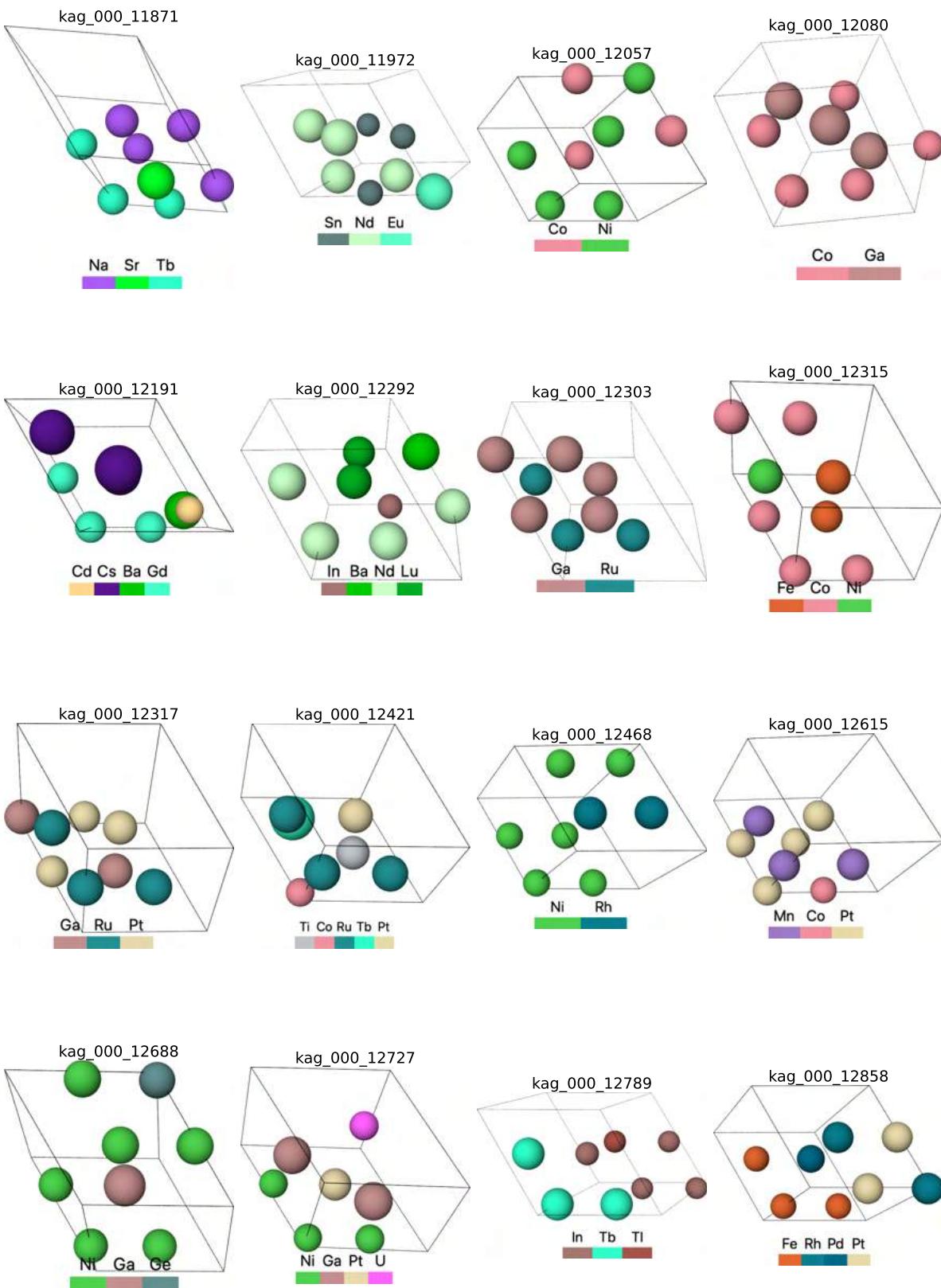


Figure S91. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

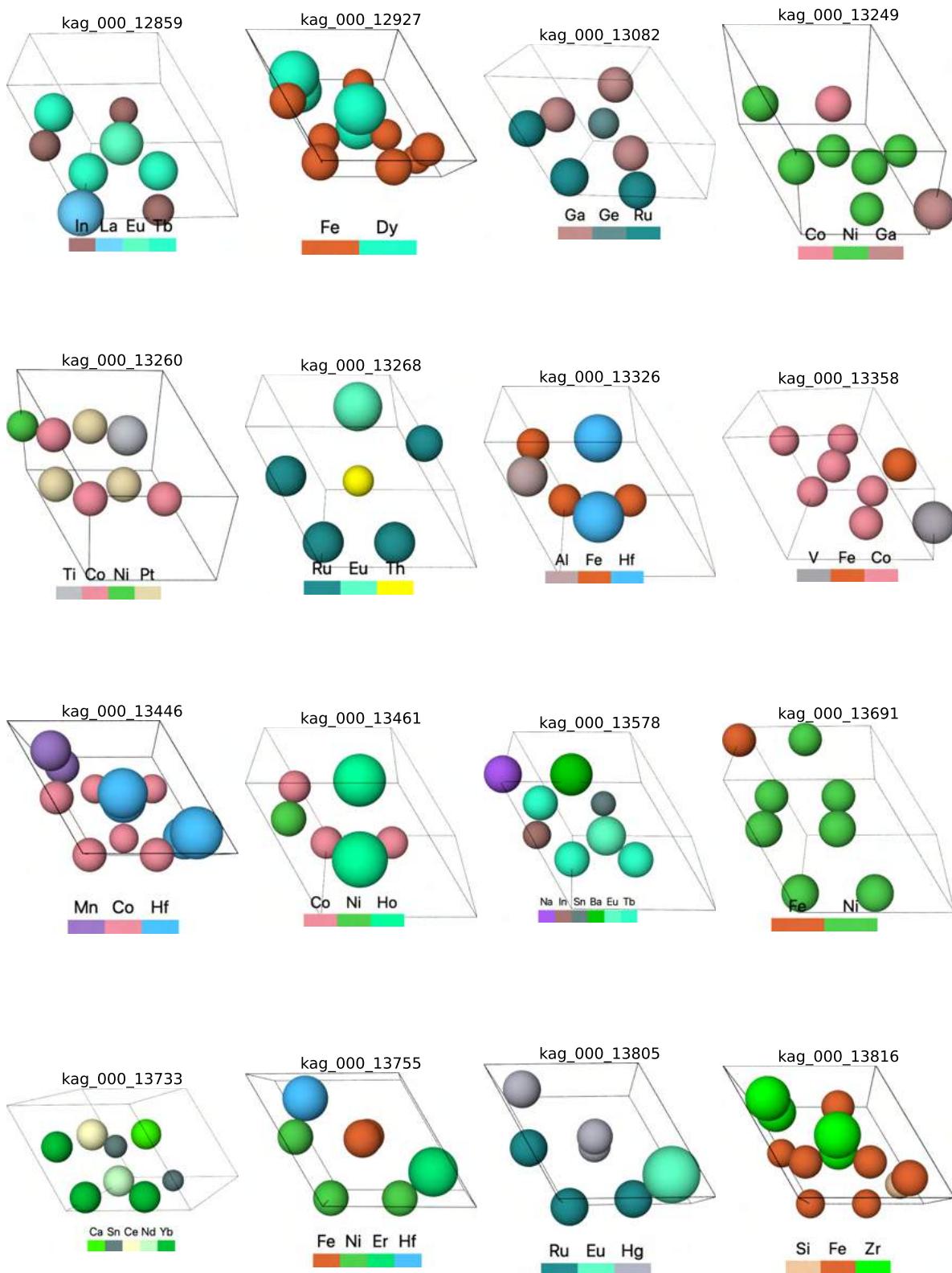


Figure S92. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

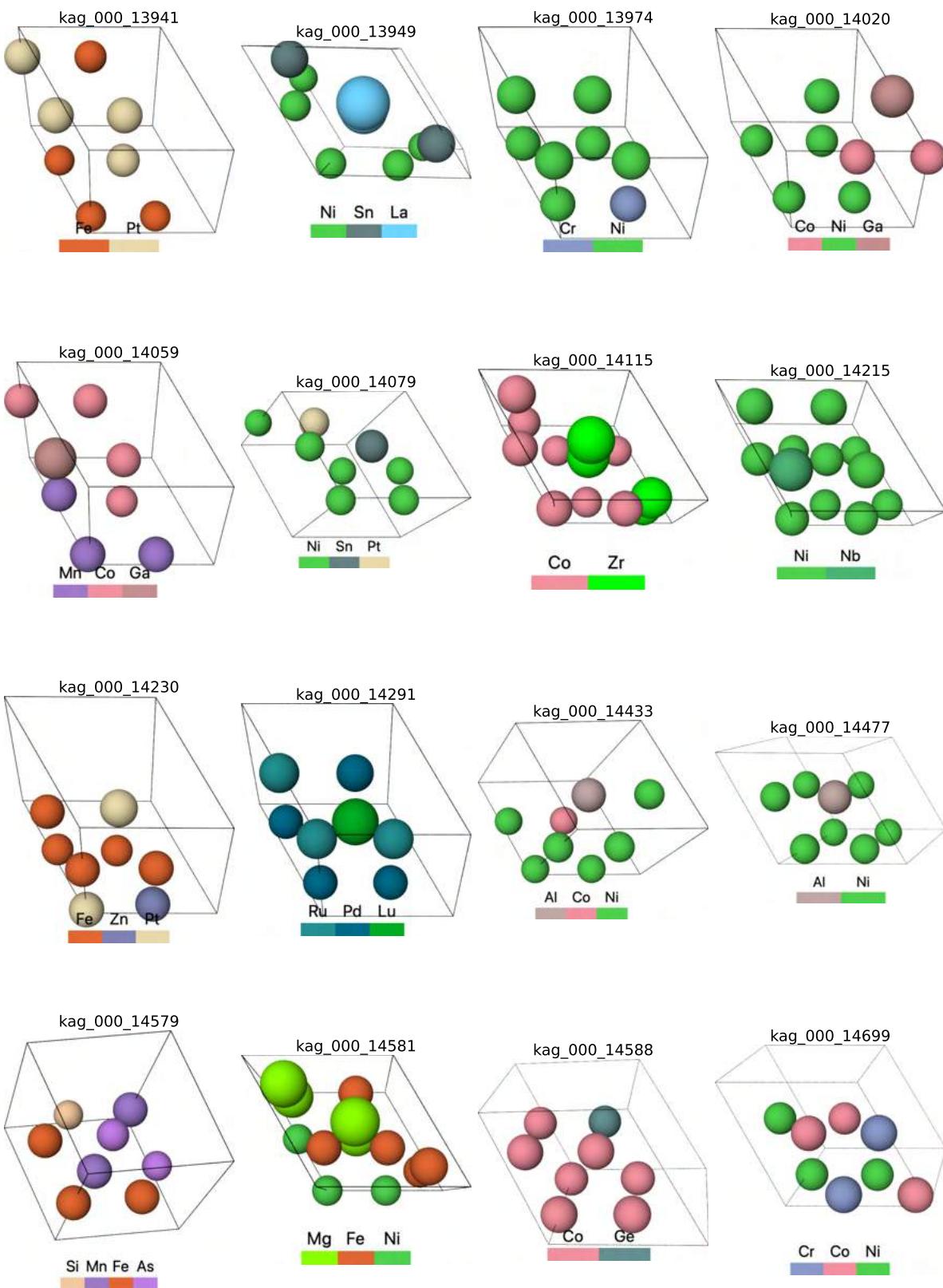


Figure S93. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

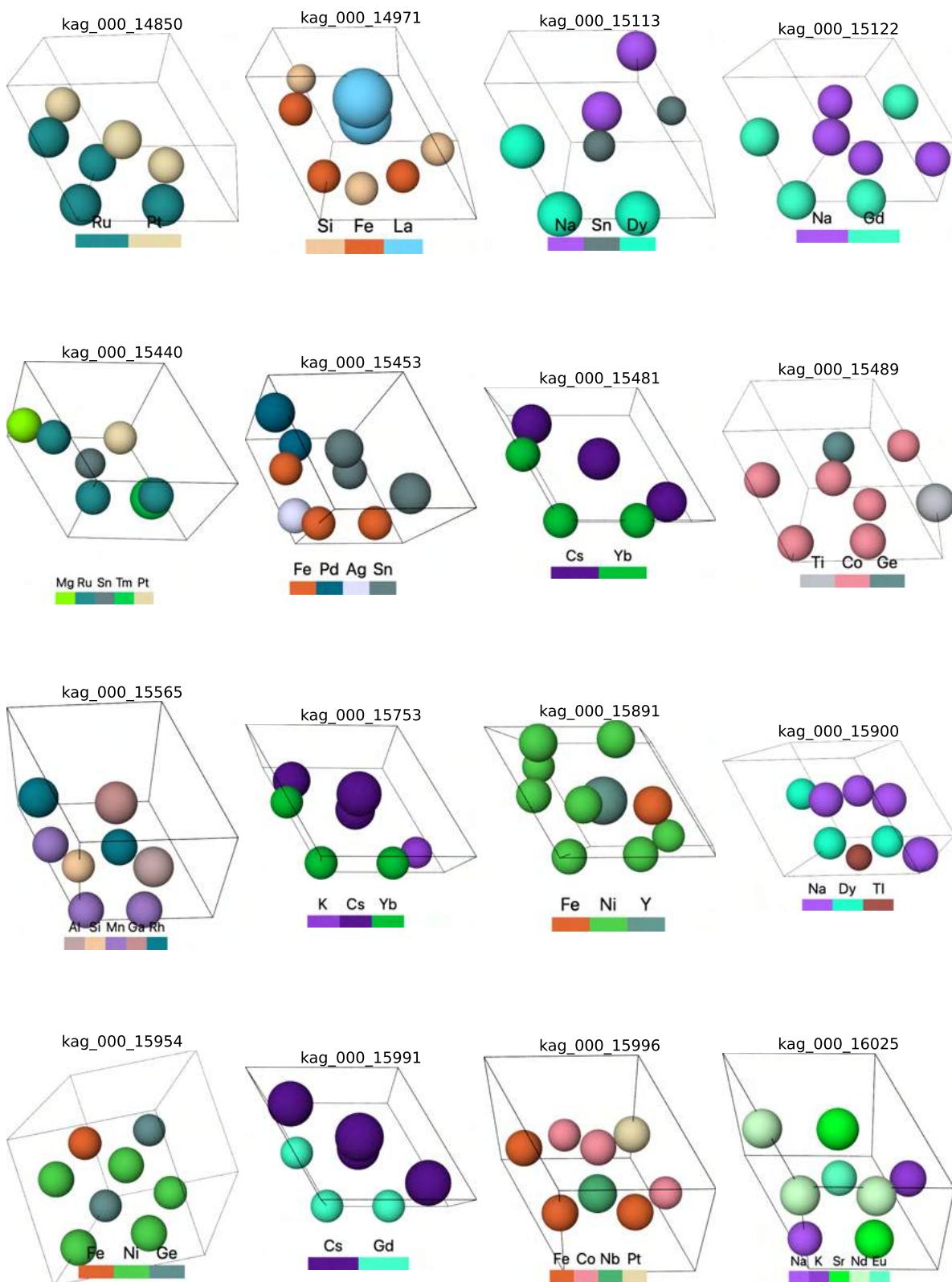


Figure S94. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

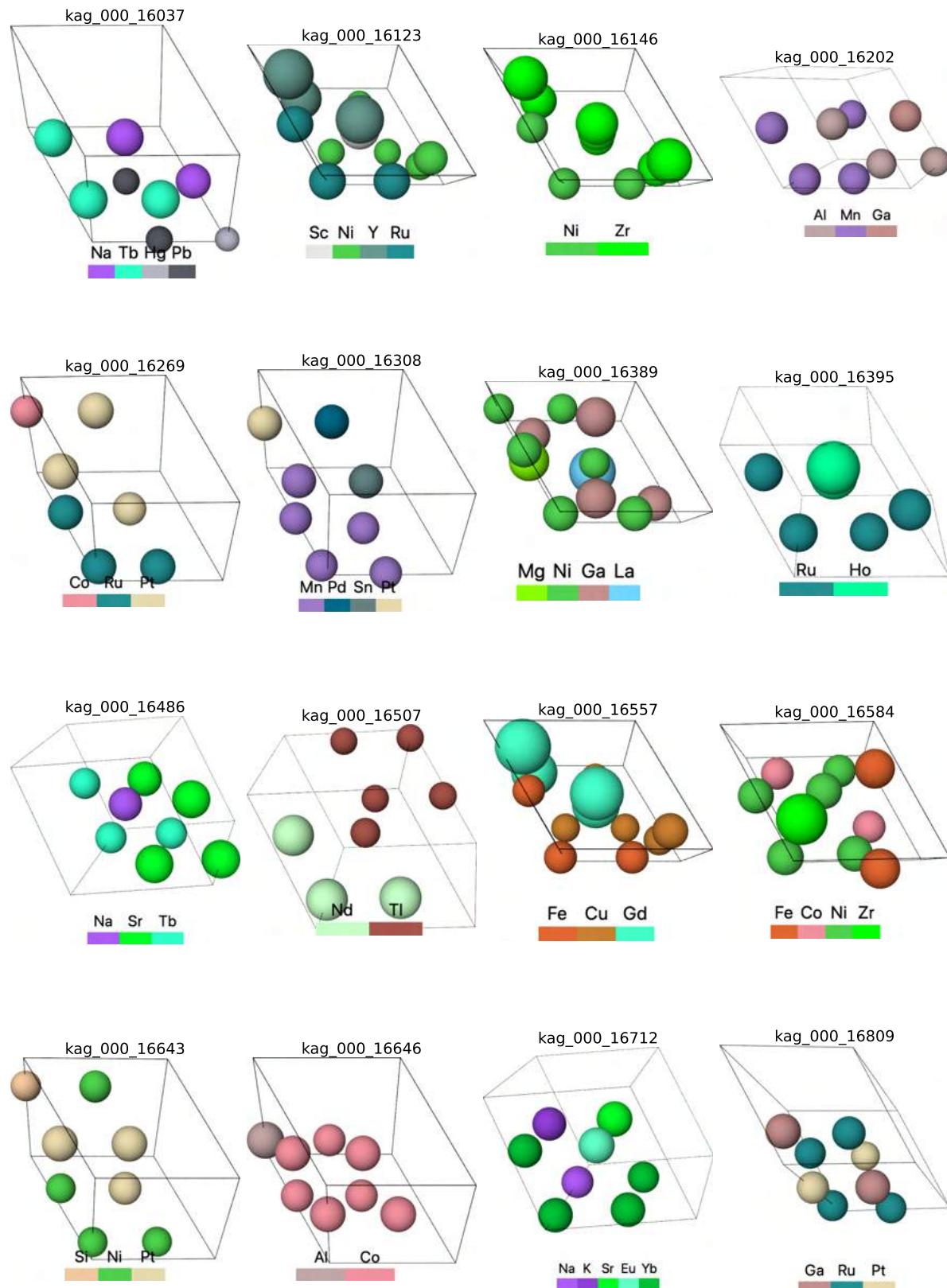


Figure S95. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

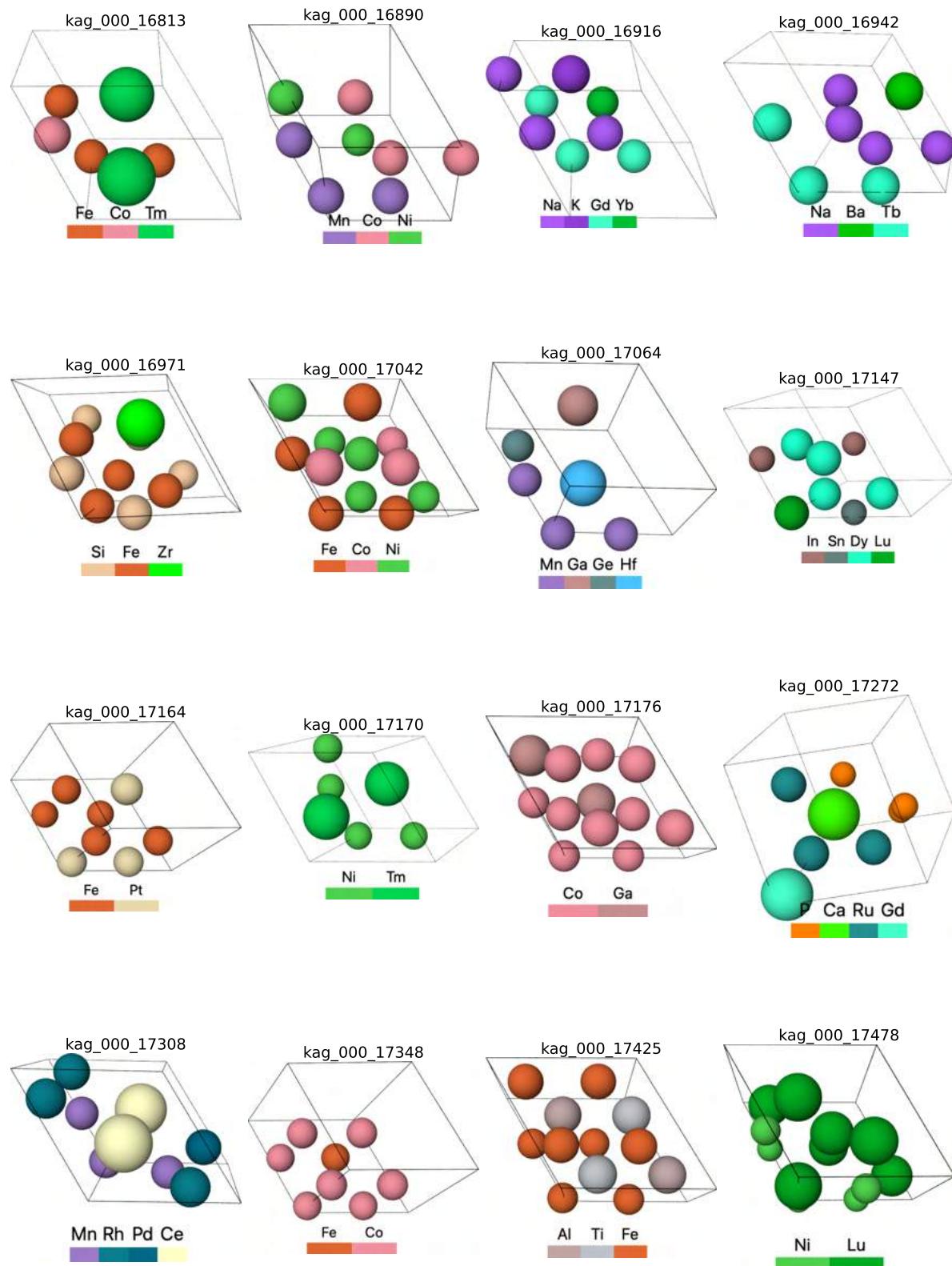


Figure S96. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

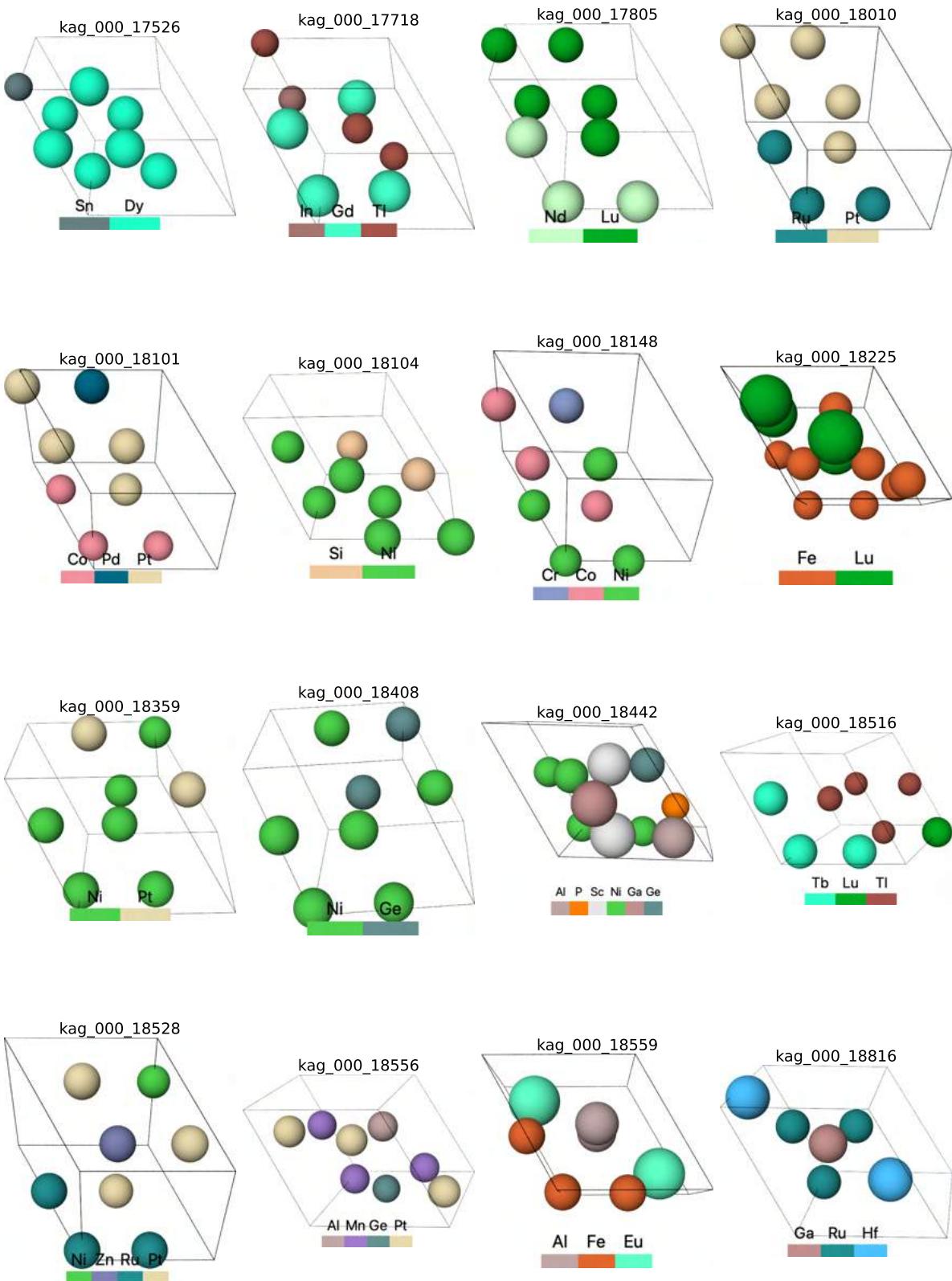


Figure S97. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

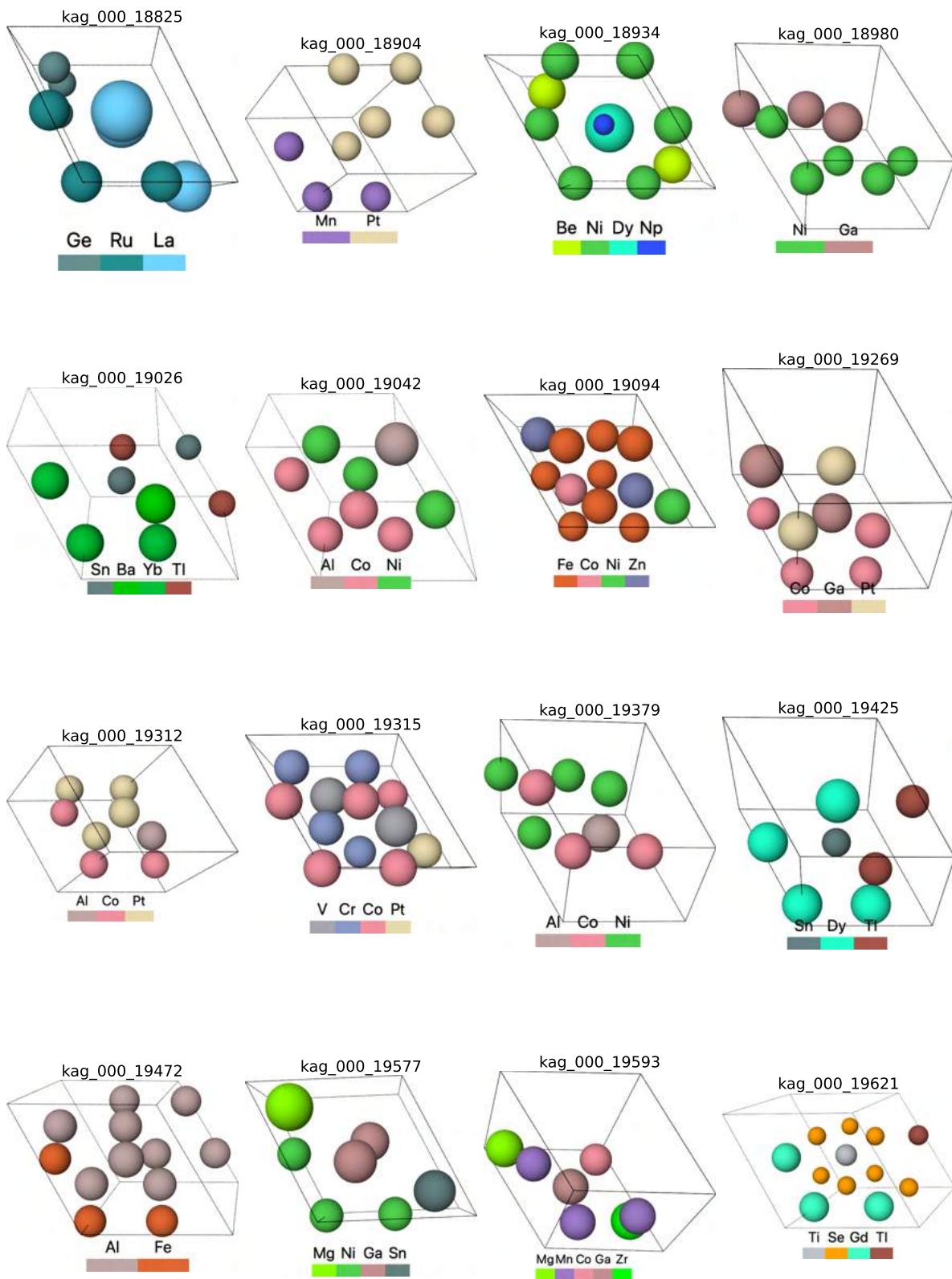


Figure S98. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

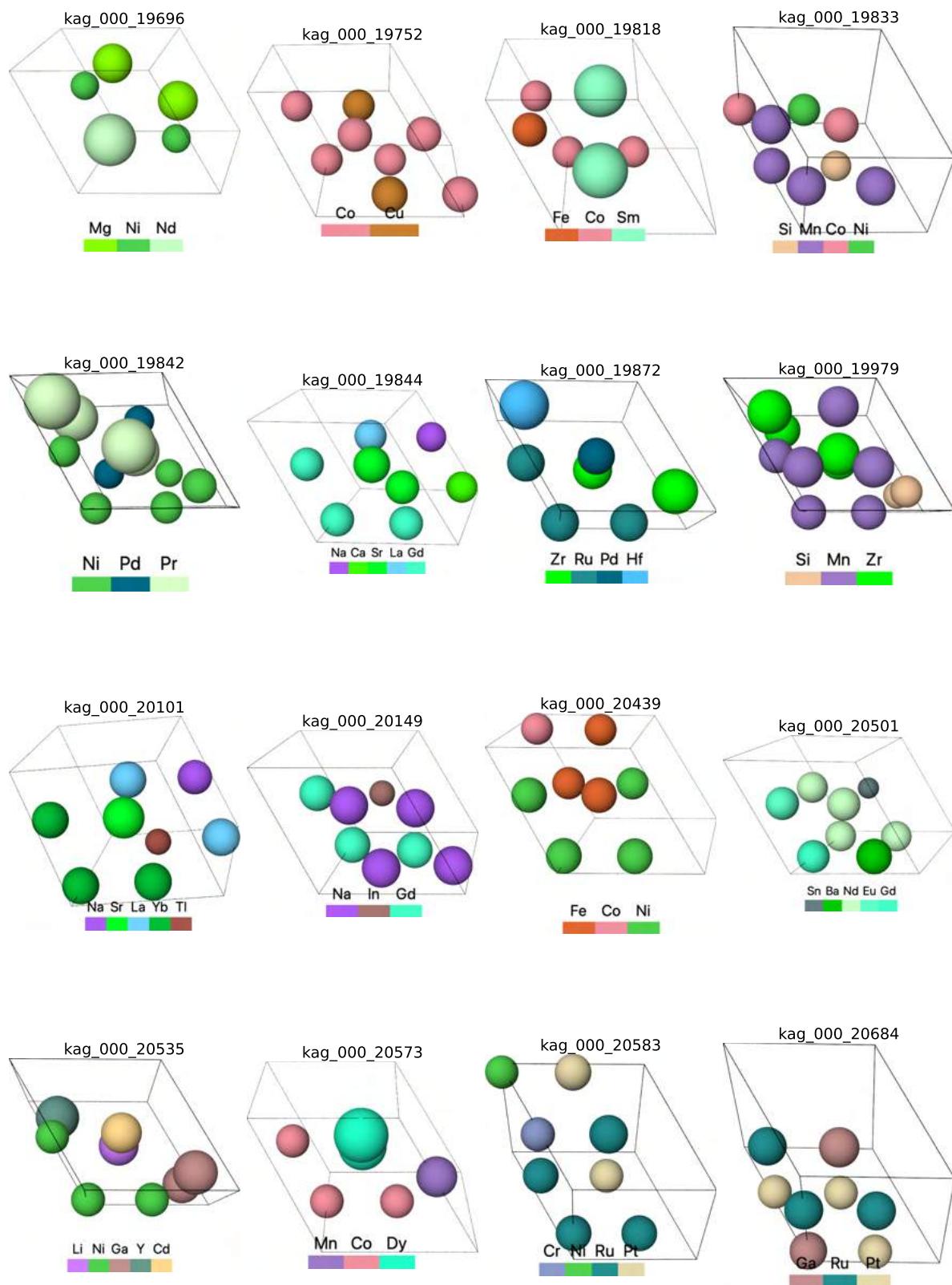


Figure S99. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

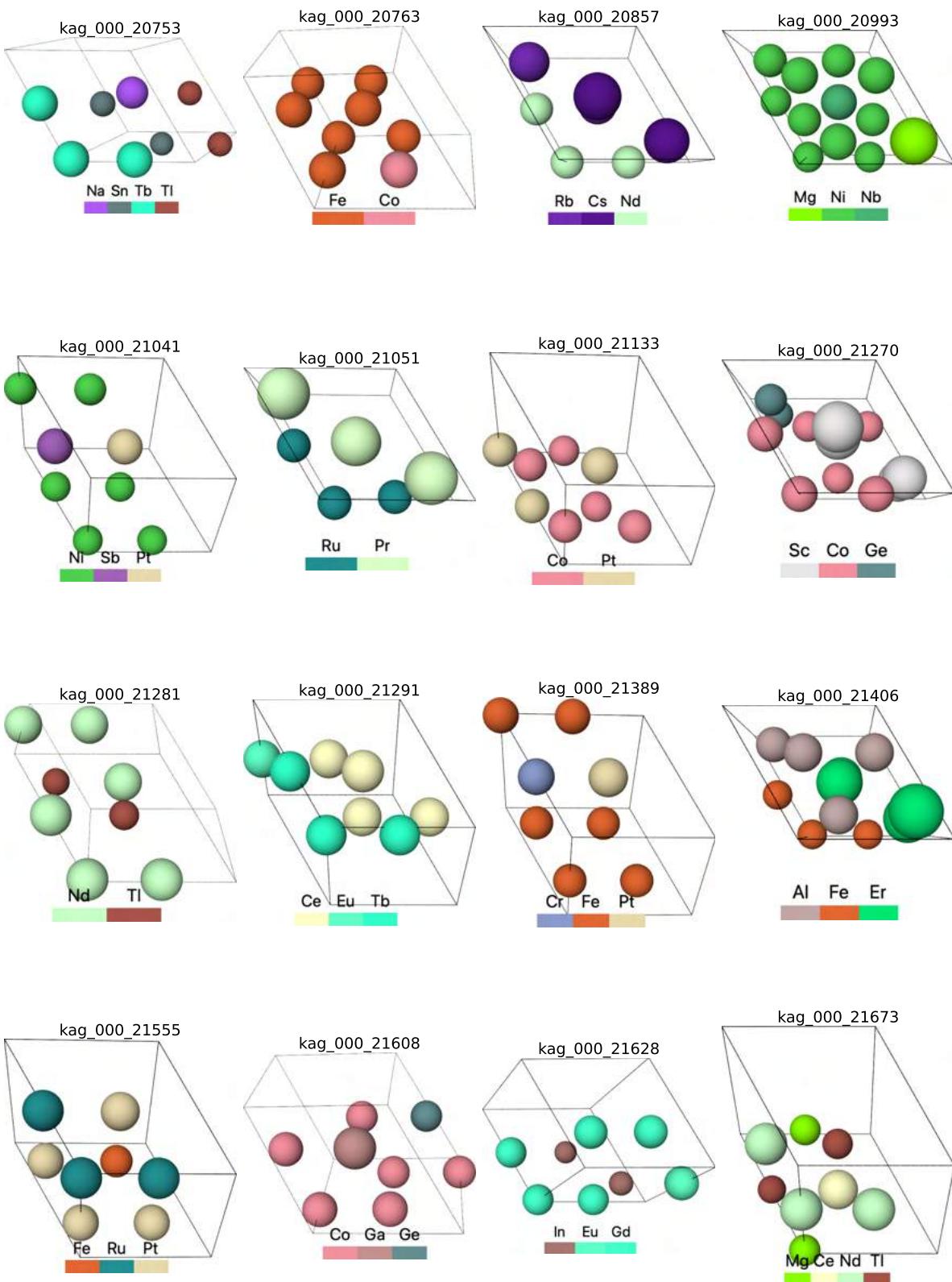


Figure S100. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

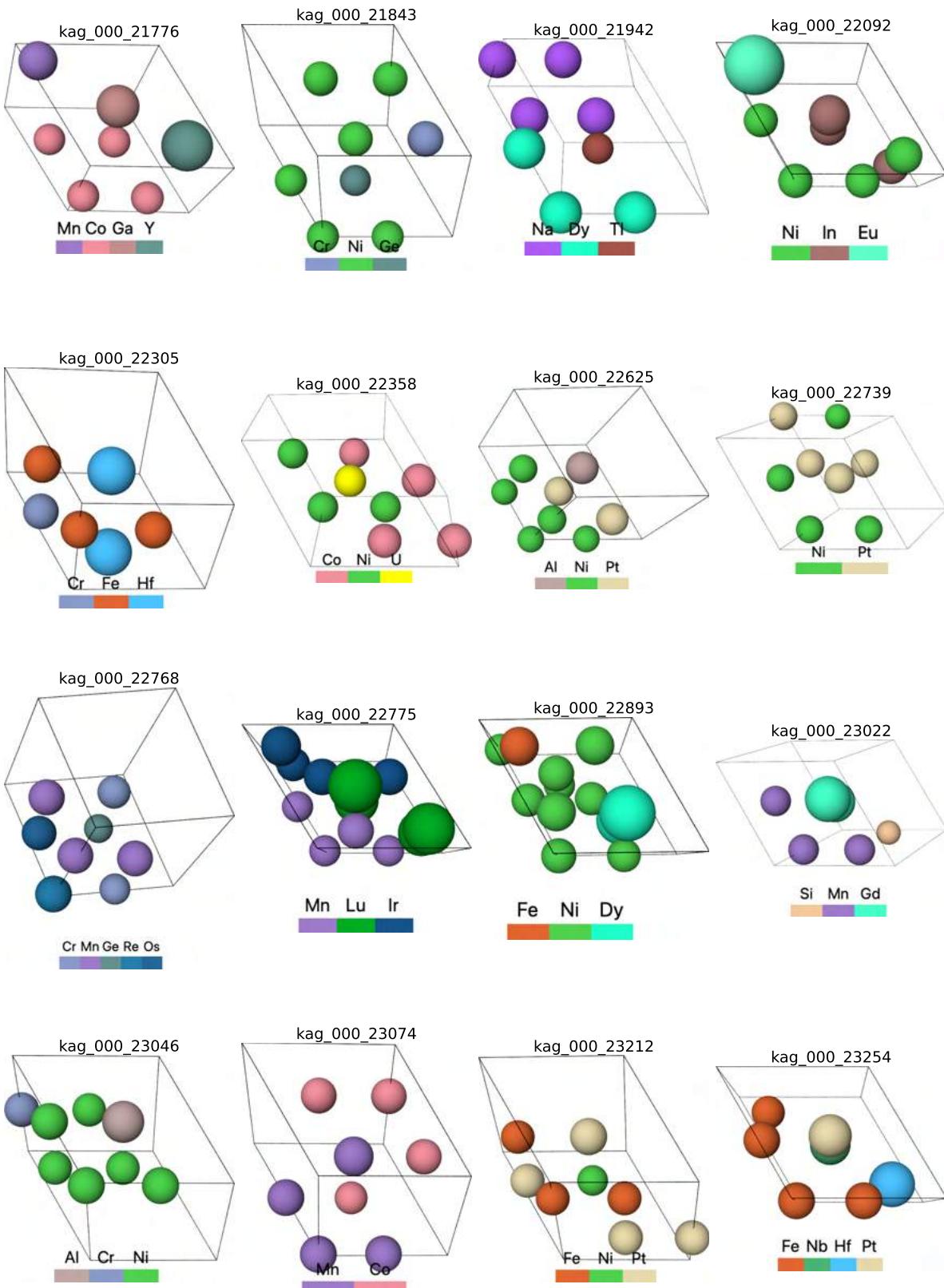


Figure S101. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

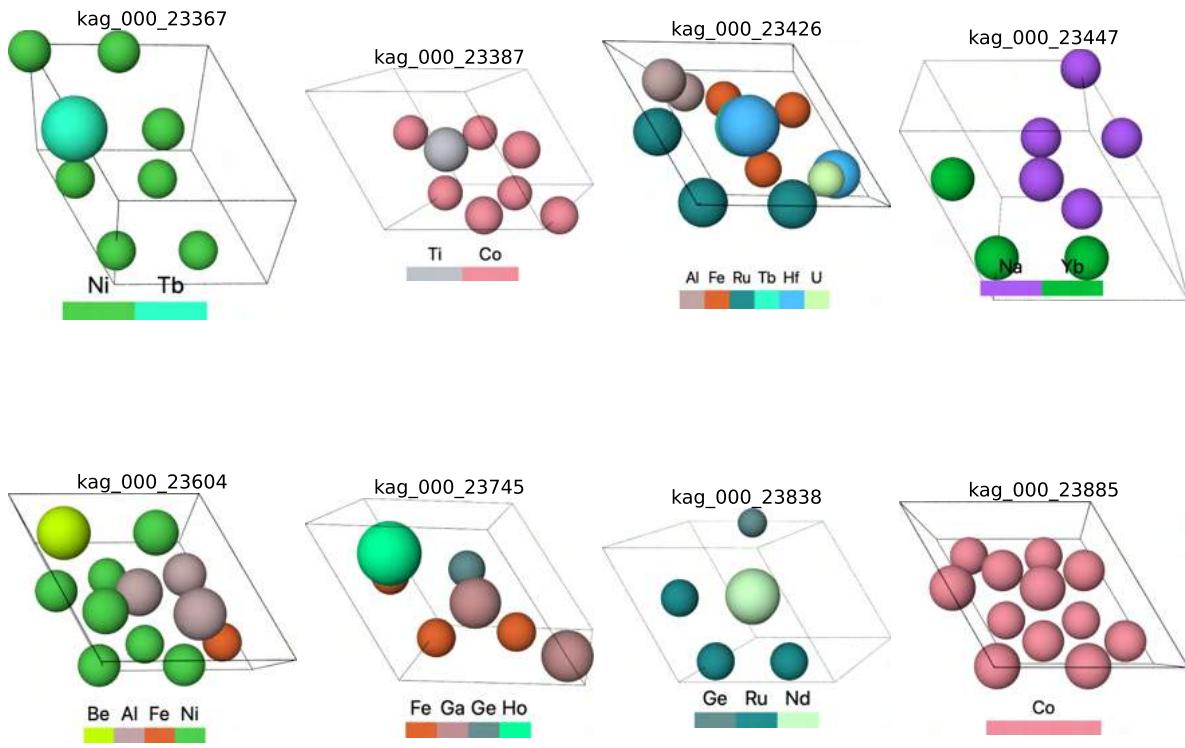


Figure S102. Generated materials with Kagome lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

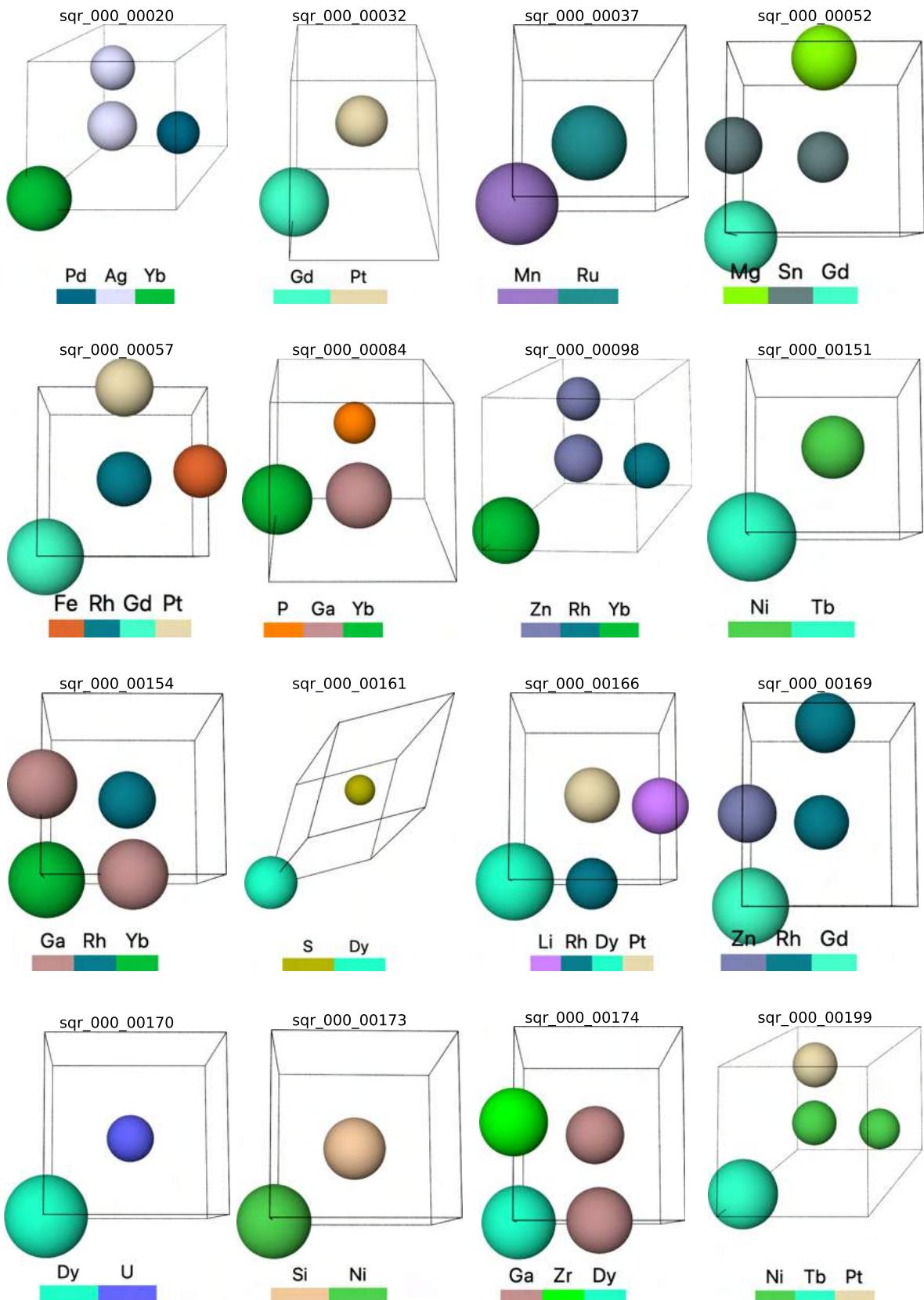


Figure S103. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

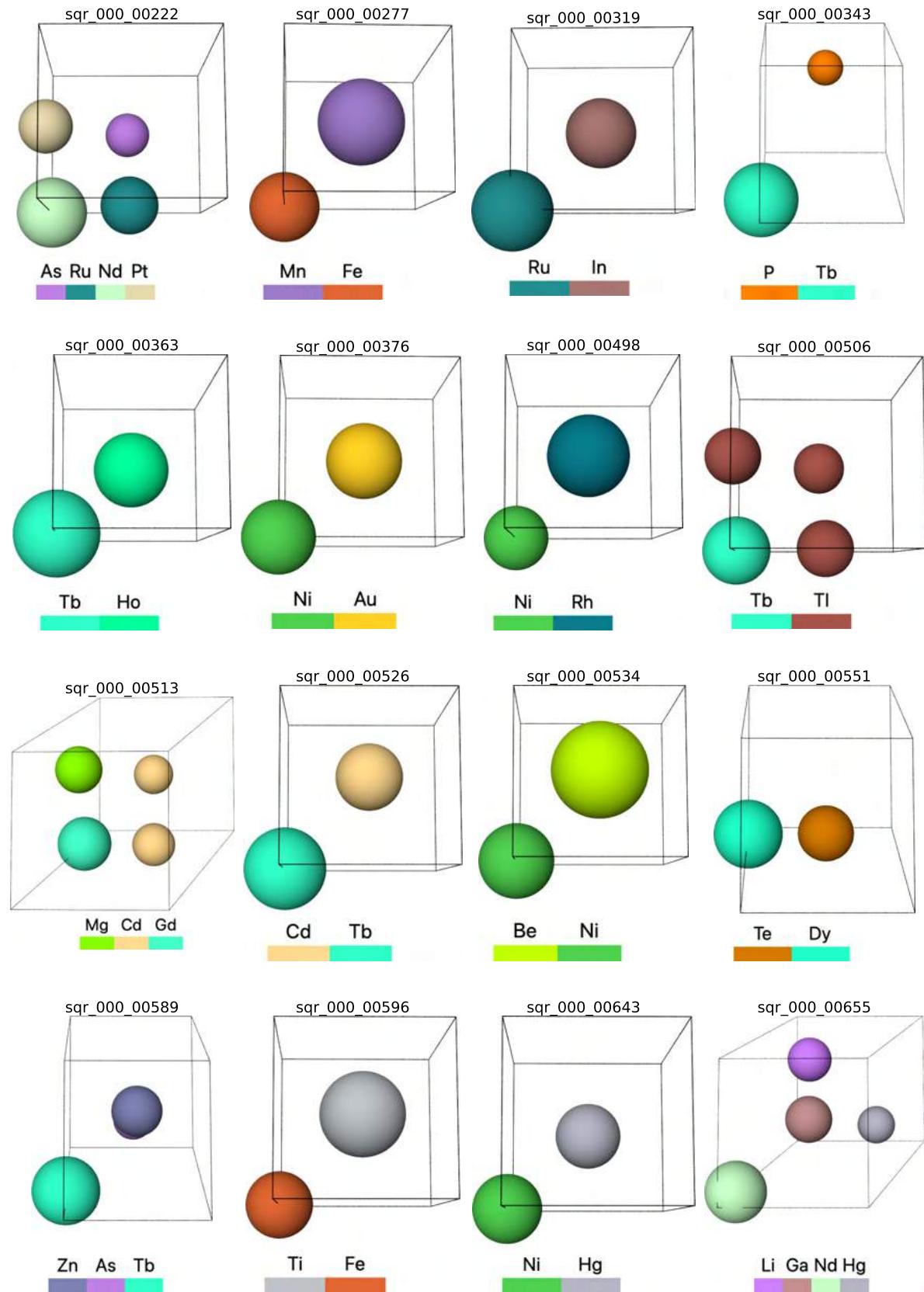


Figure S104. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

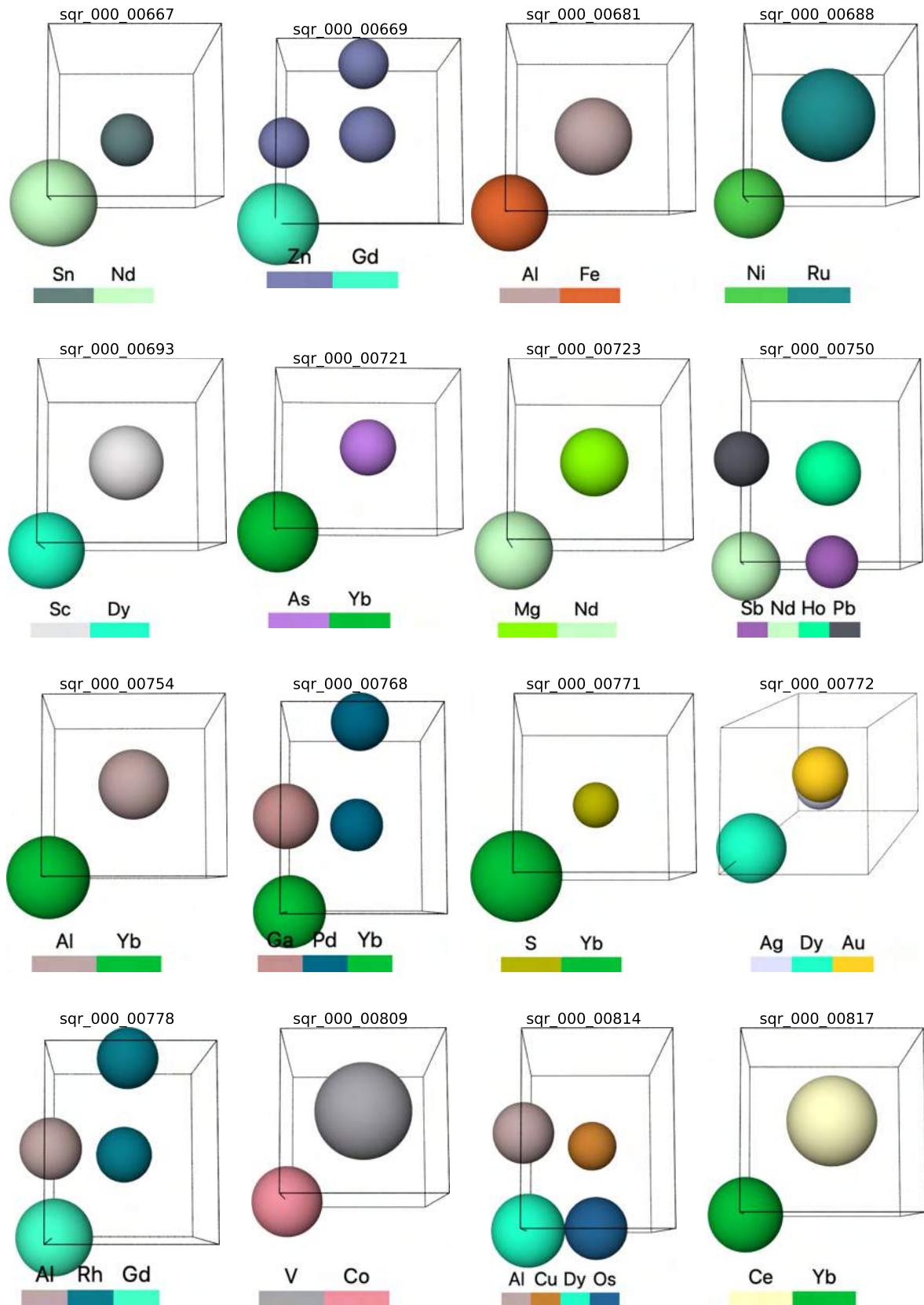


Figure S105. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

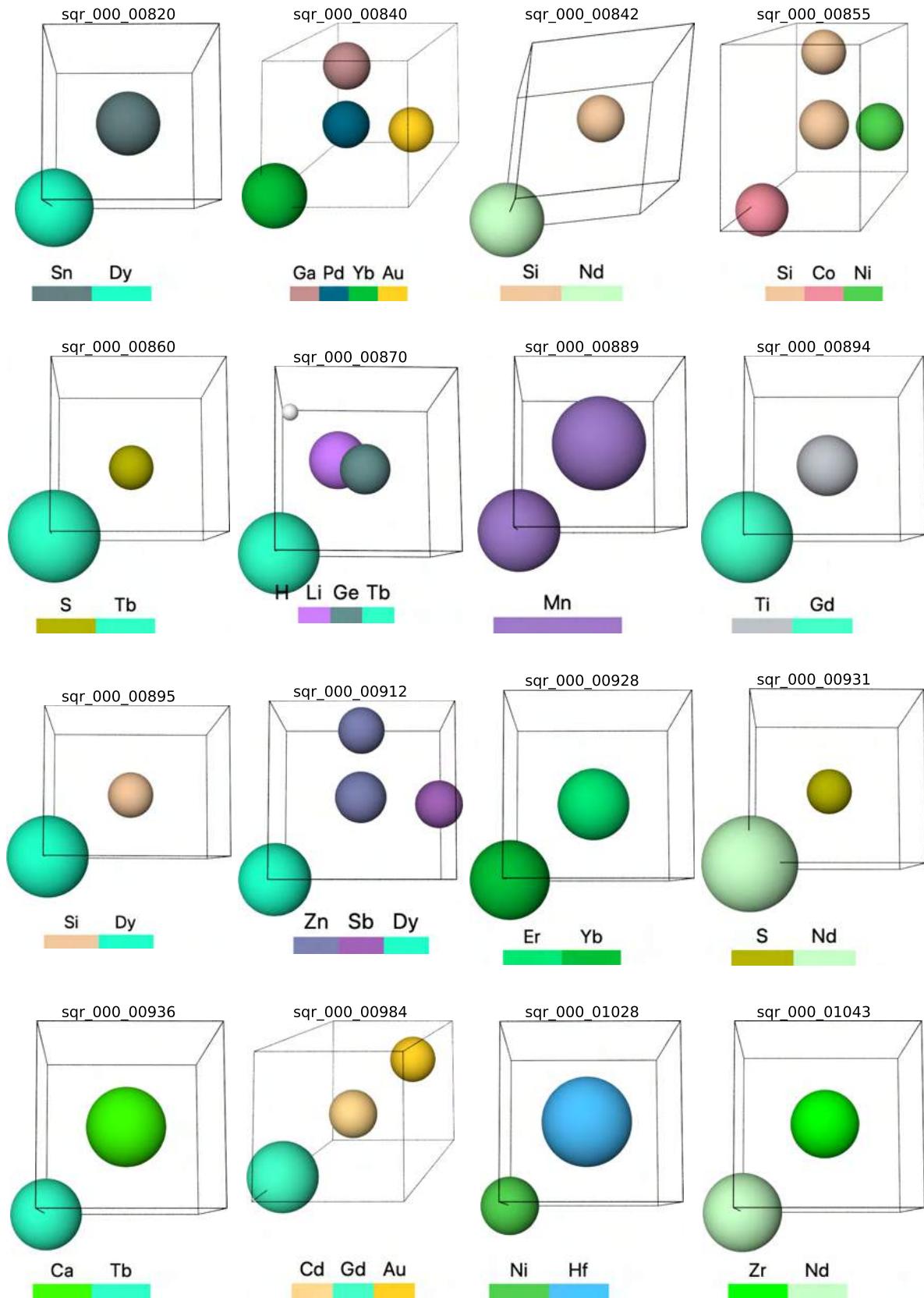


Figure S106. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

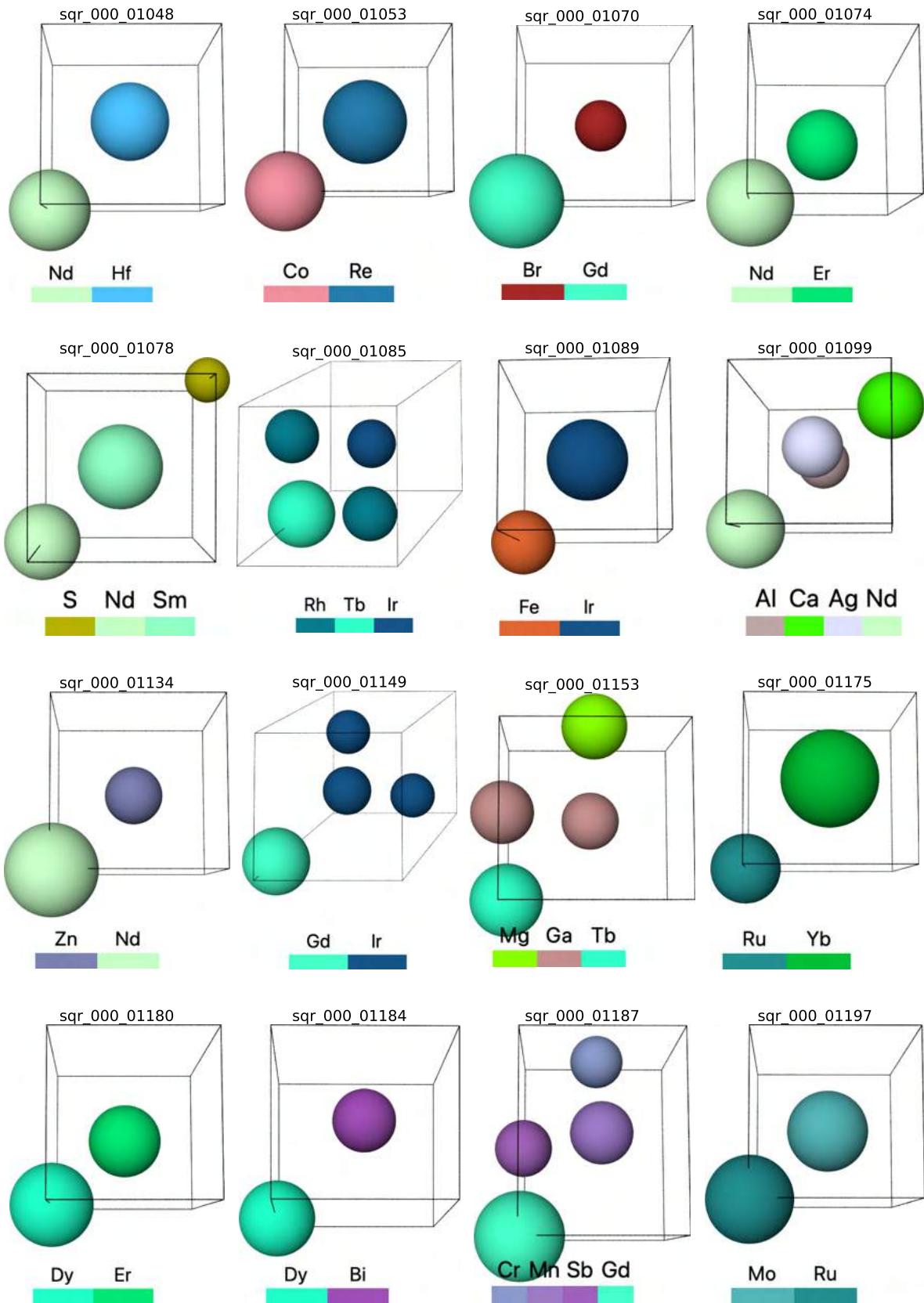


Figure S107. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

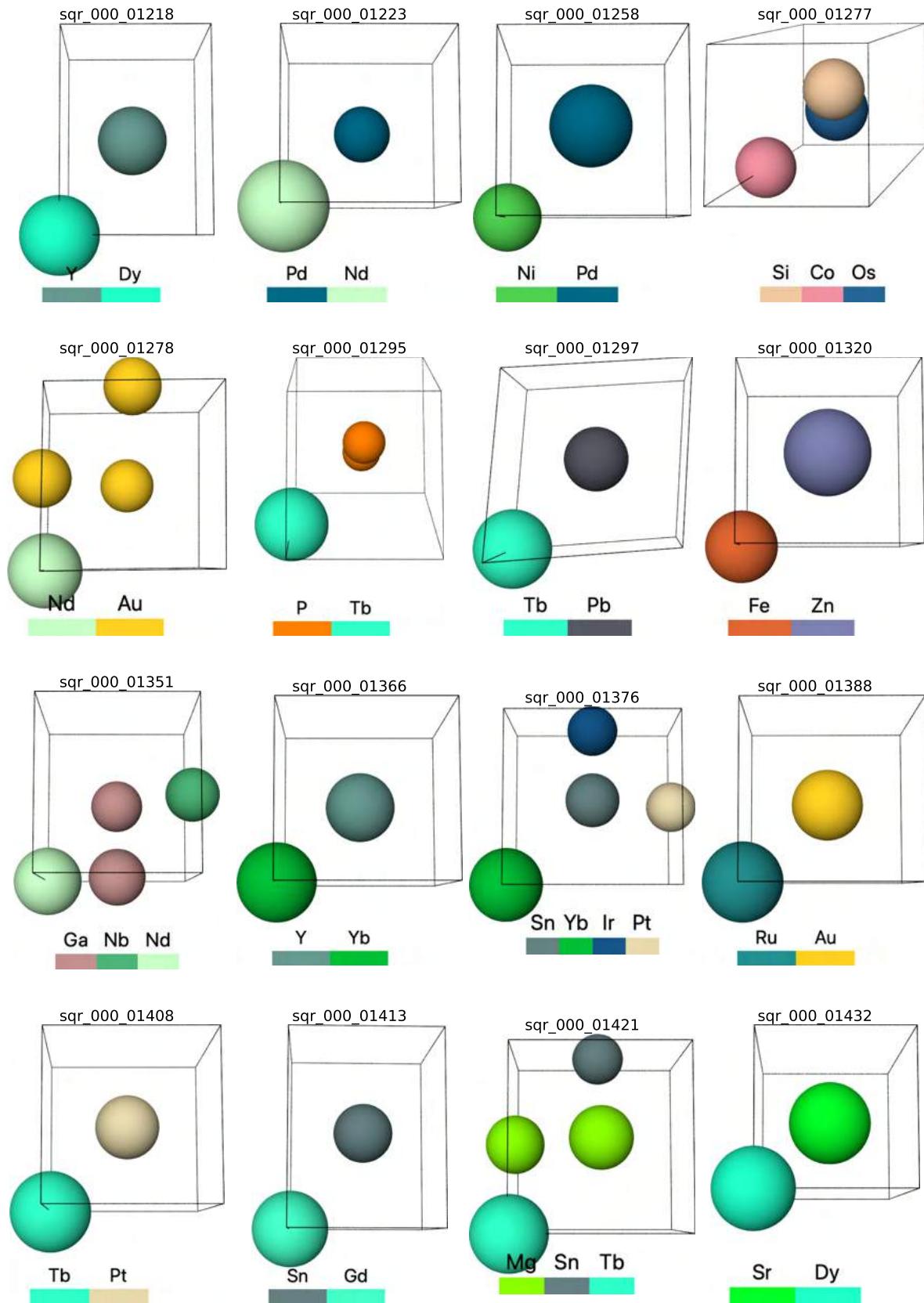


Figure S108. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

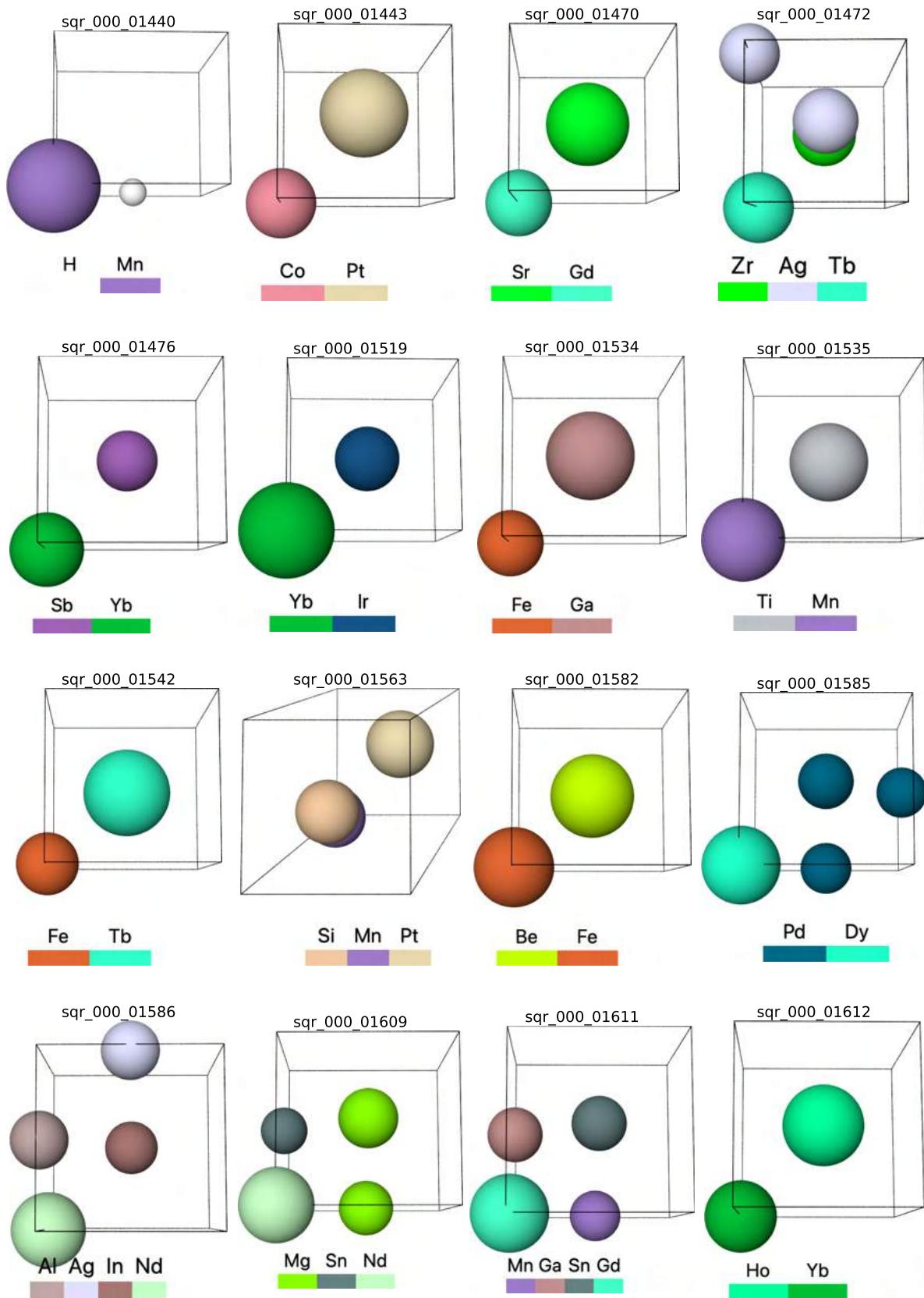


Figure S109. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

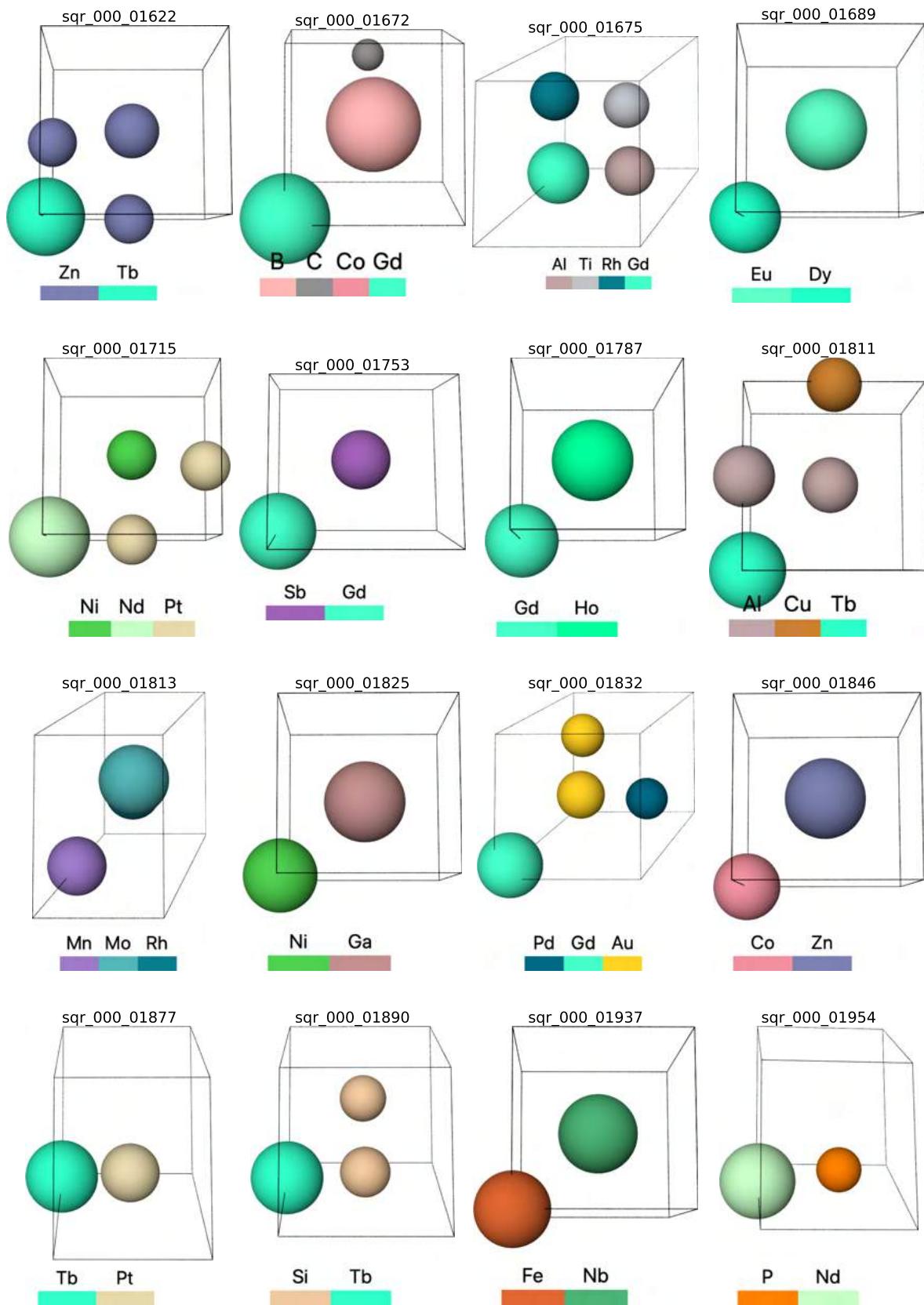


Figure S110. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

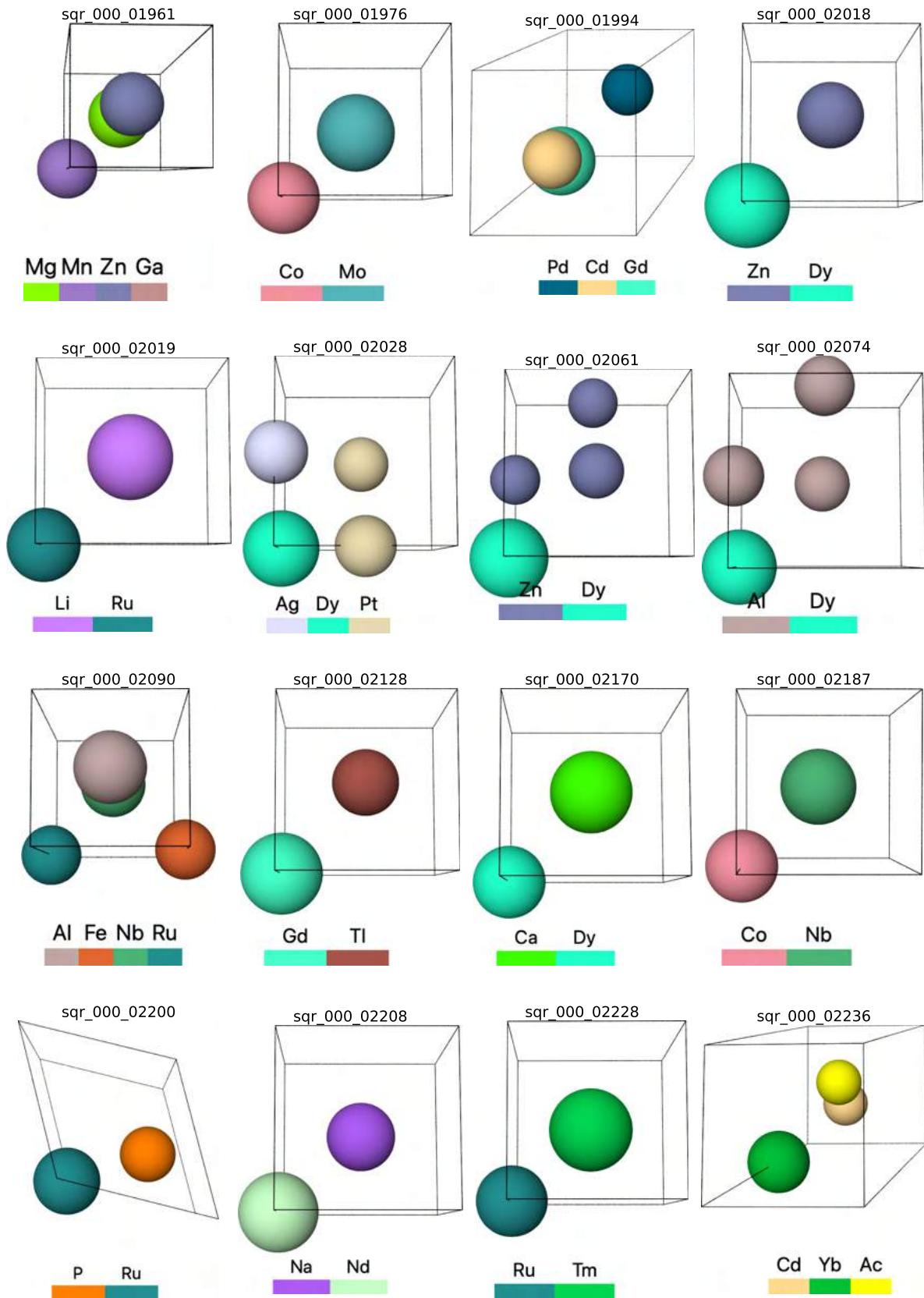


Figure S111. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

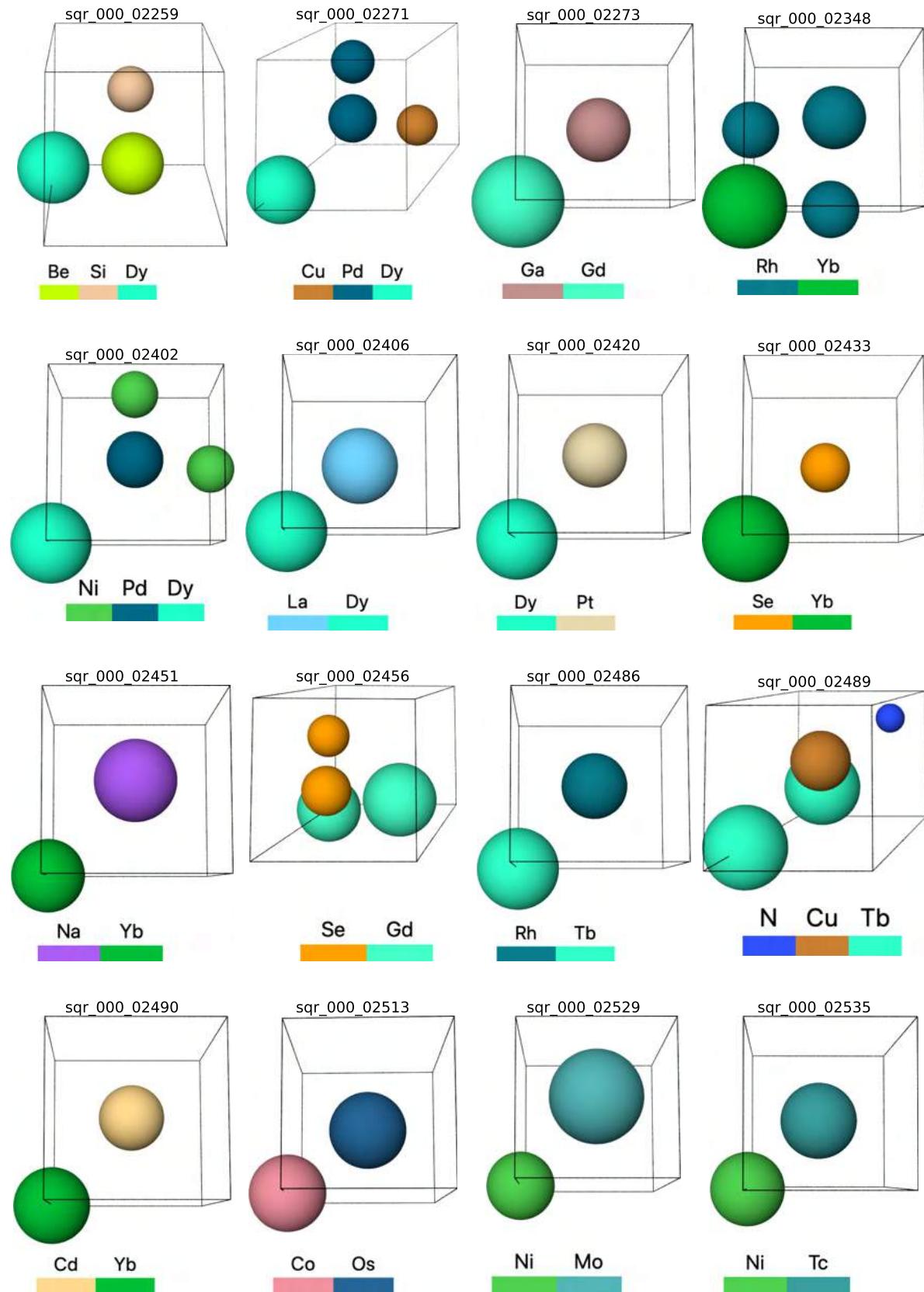


Figure S112. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

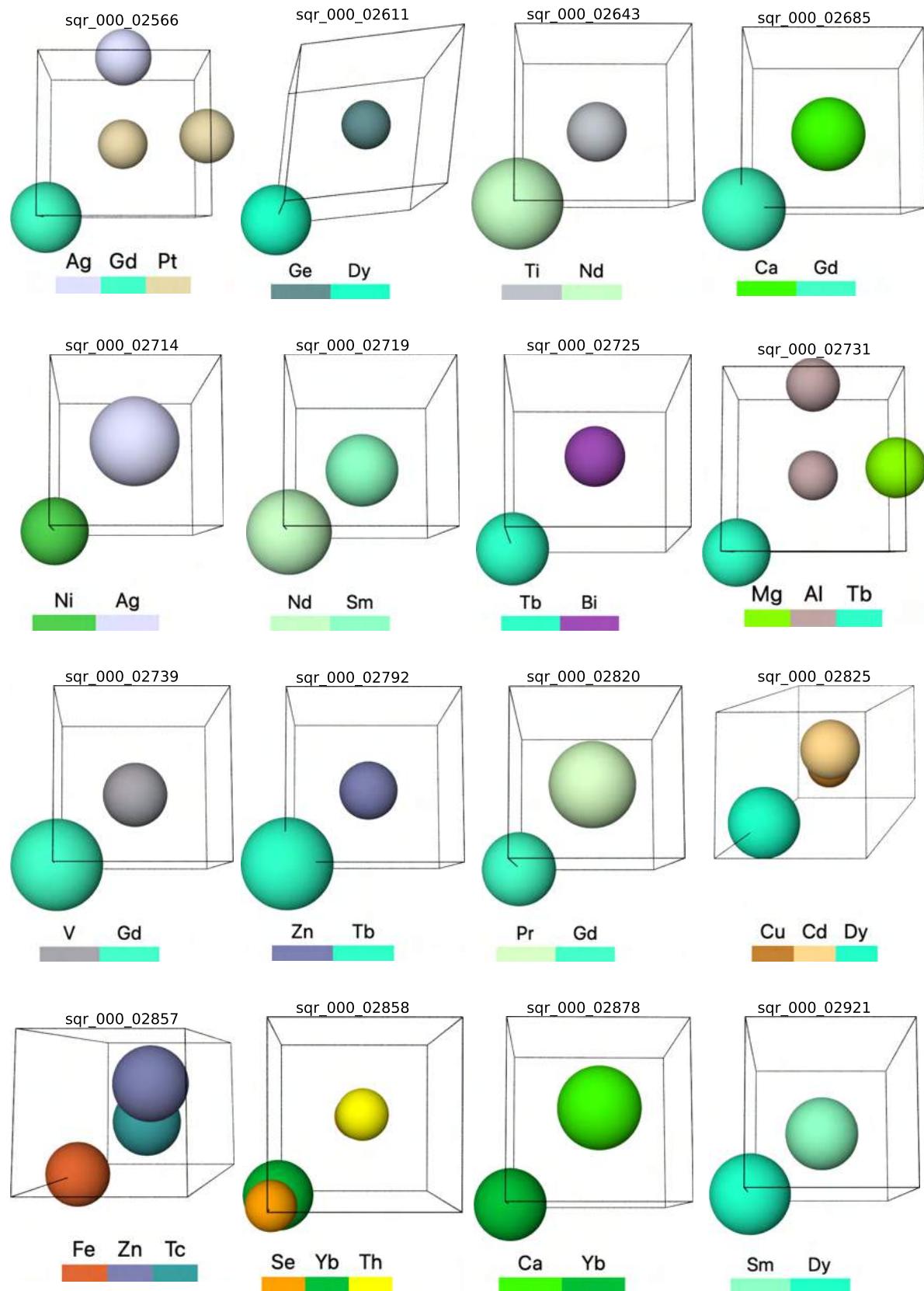


Figure S113. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

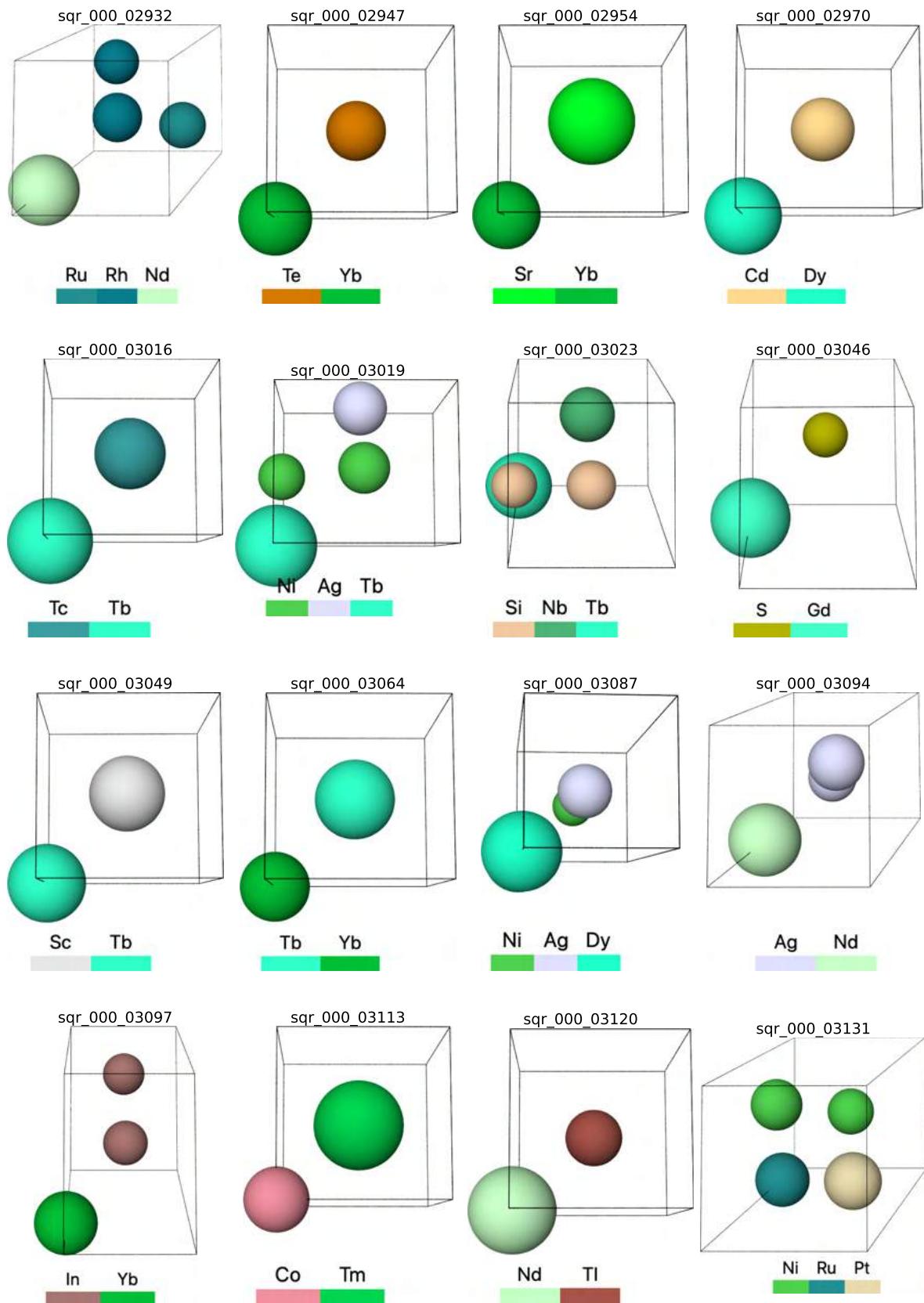


Figure S114. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

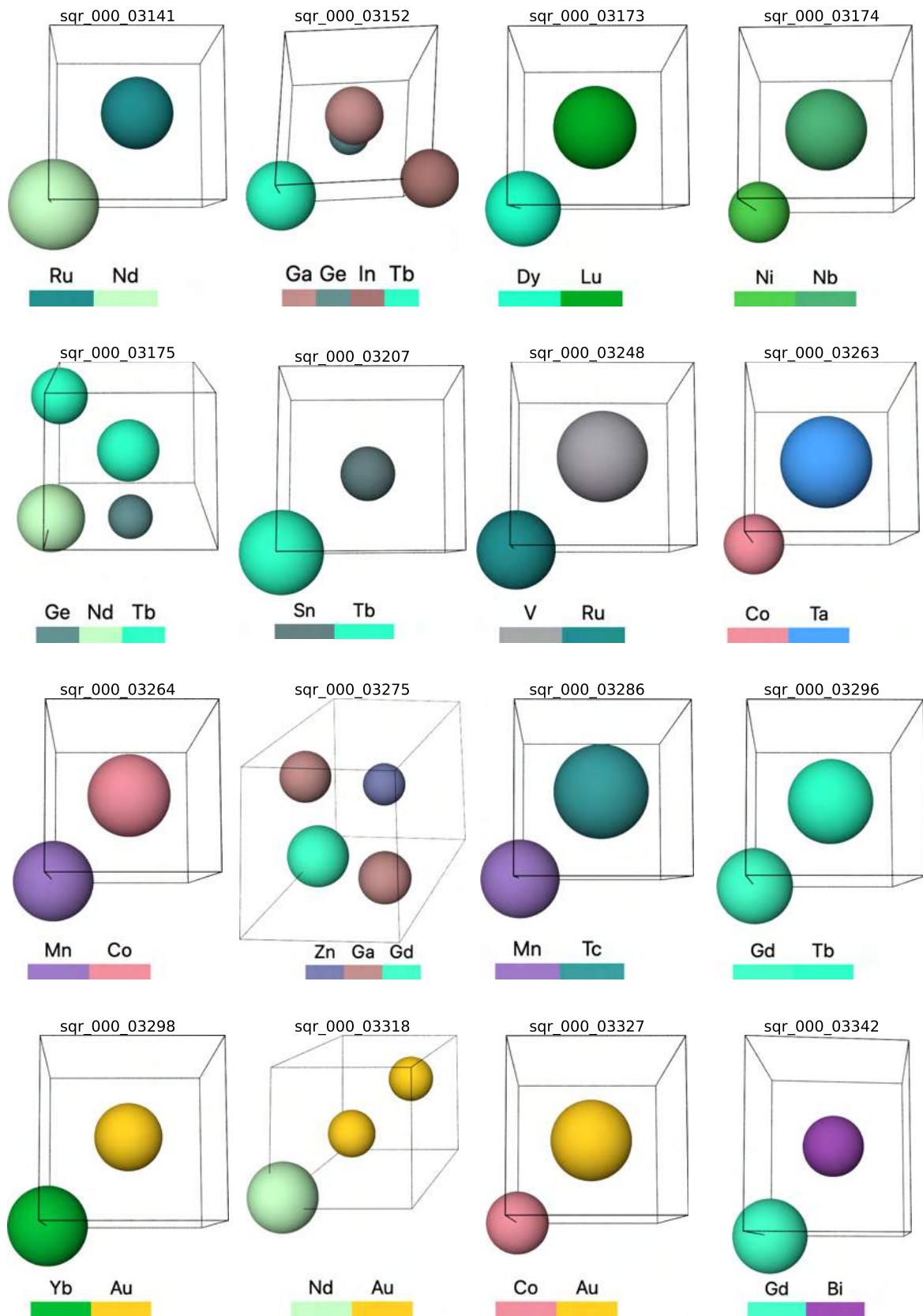


Figure S115. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

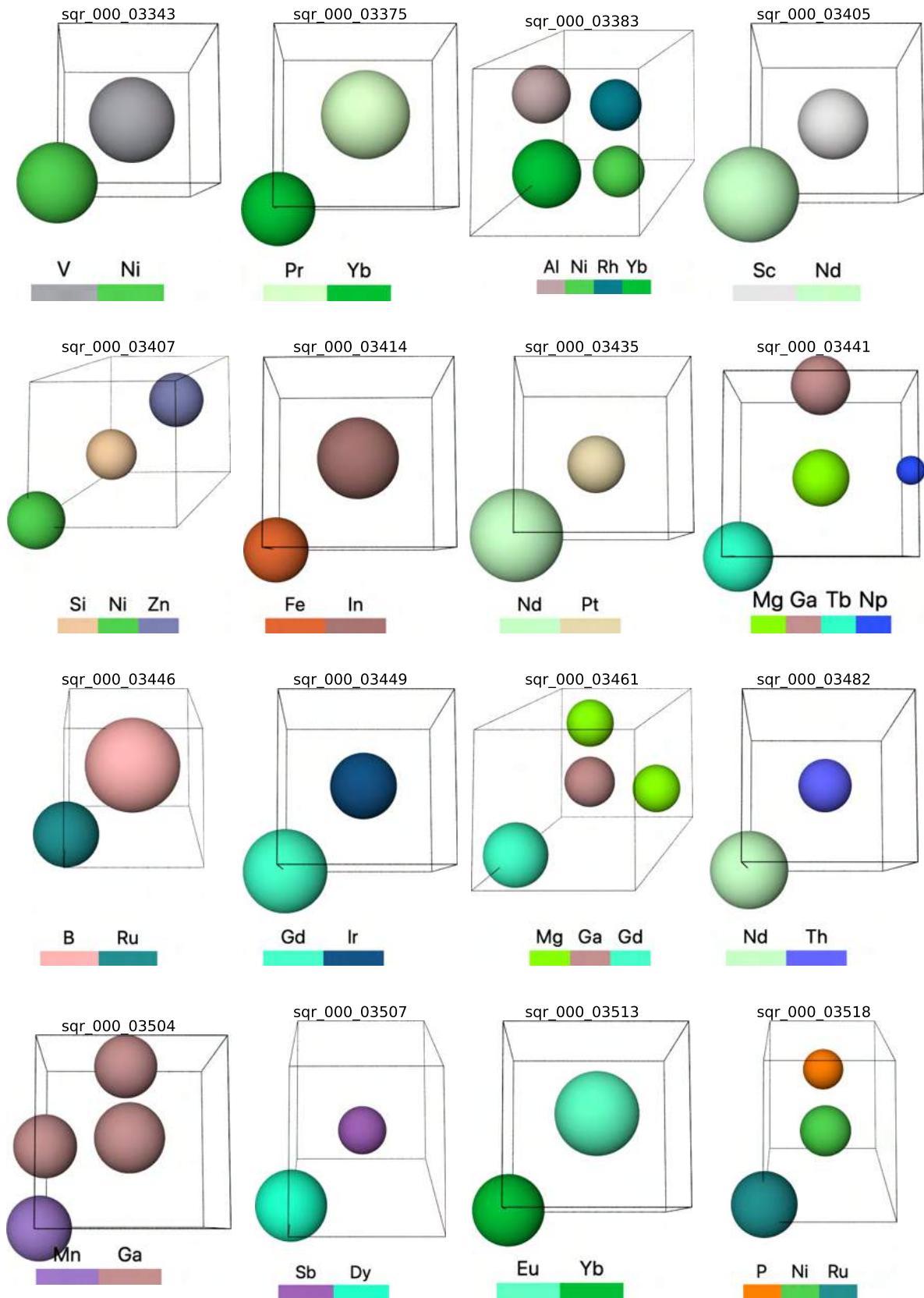


Figure S116. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

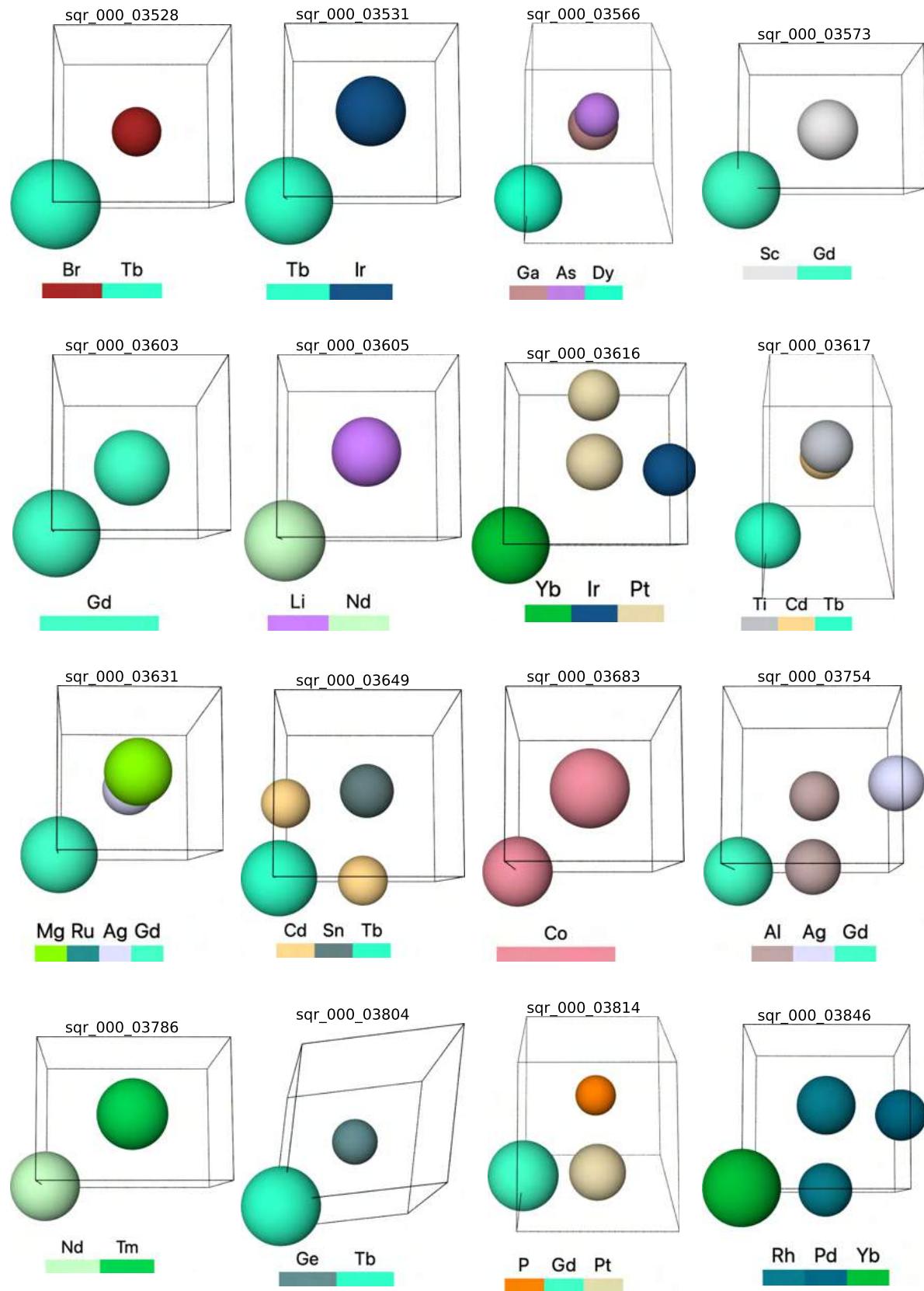


Figure S117. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

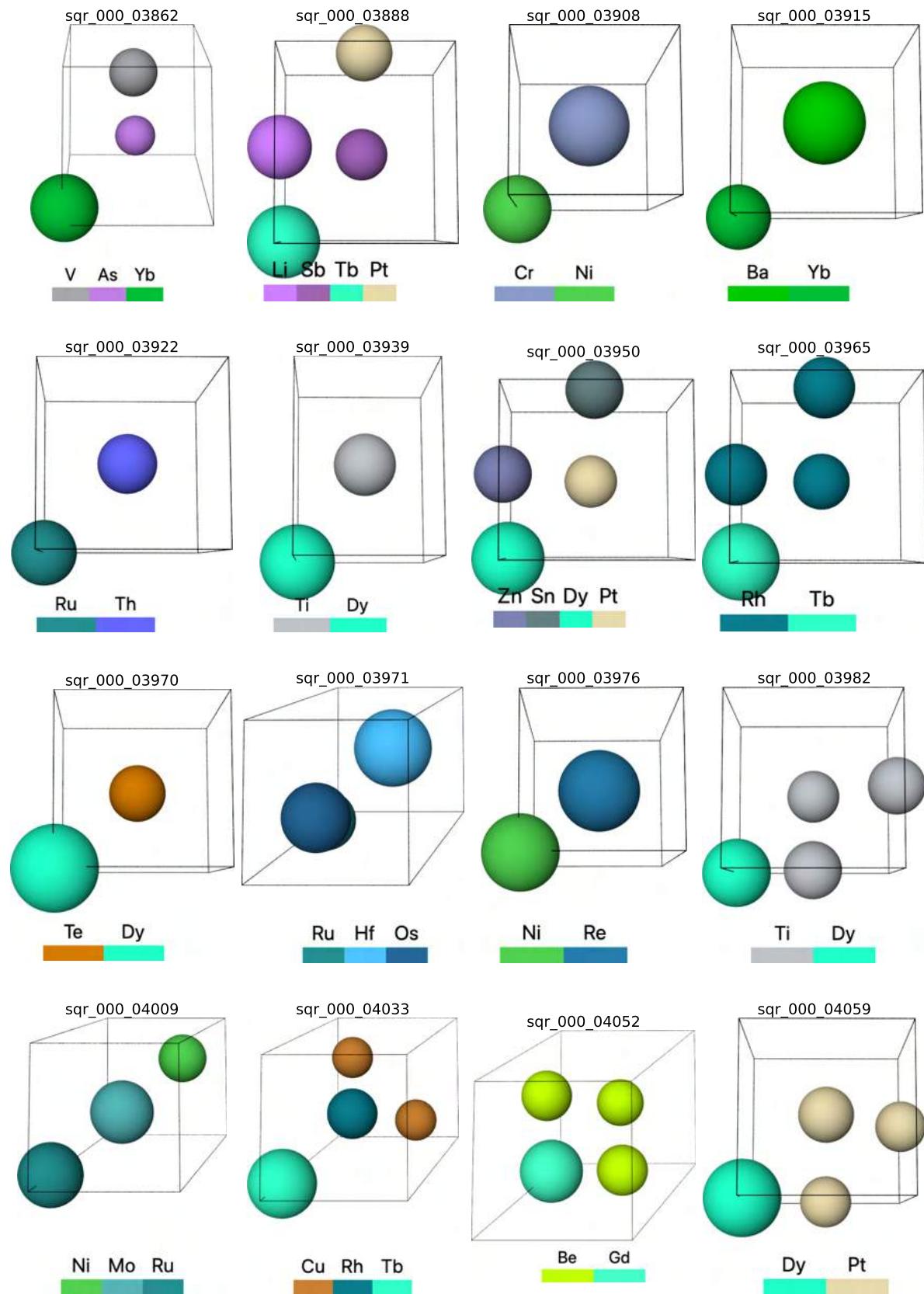


Figure S118. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

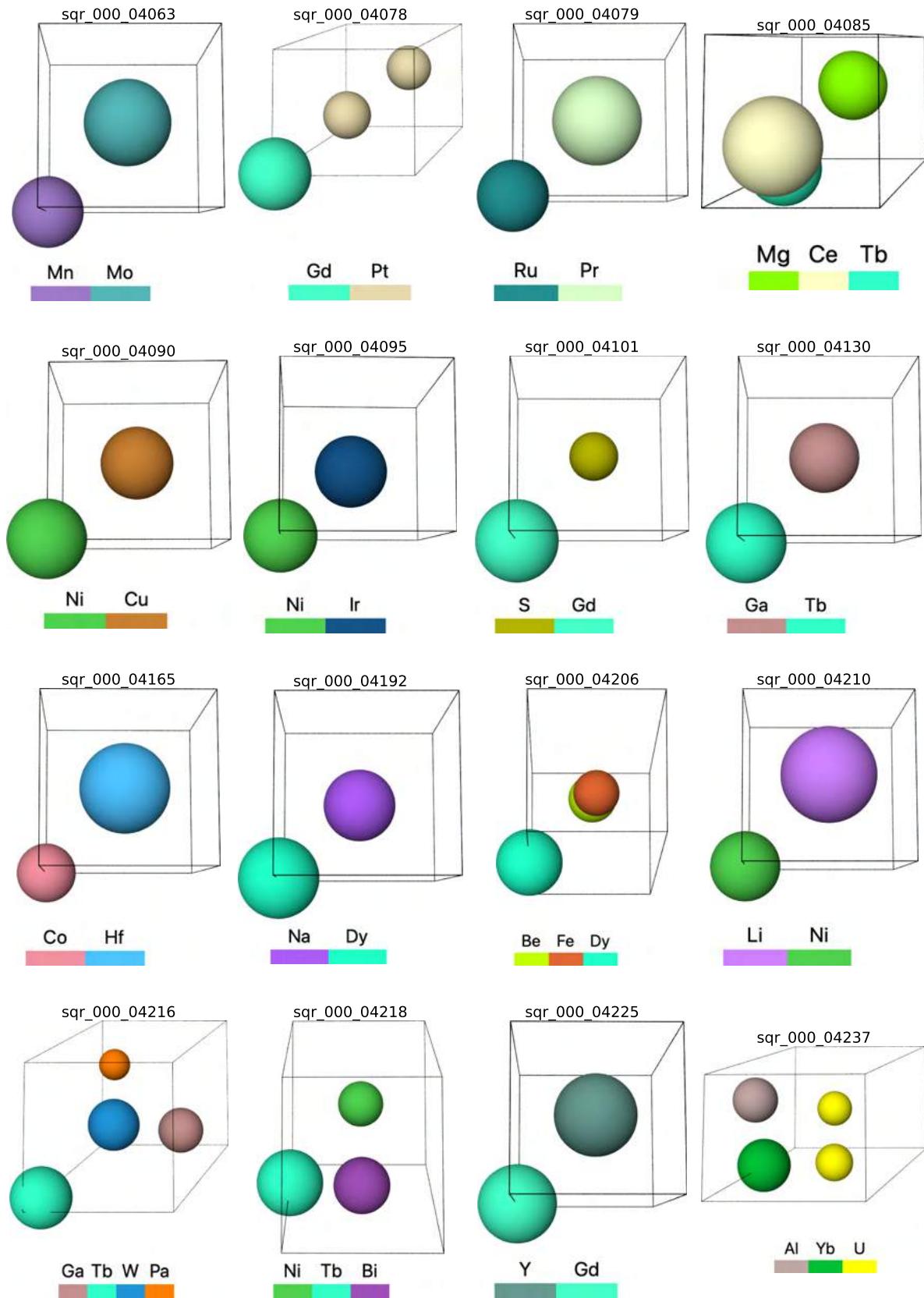


Figure S119. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

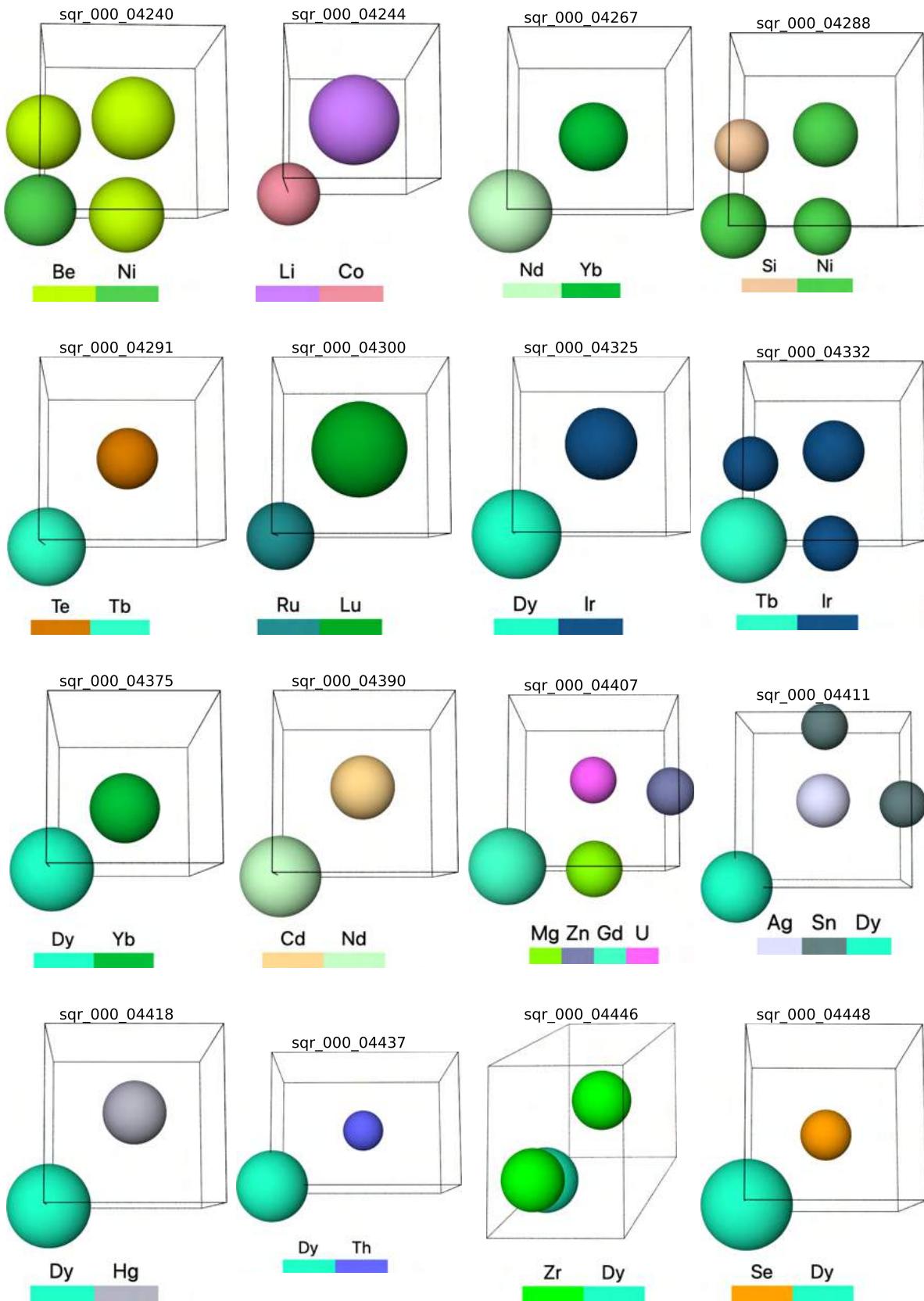


Figure S120. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

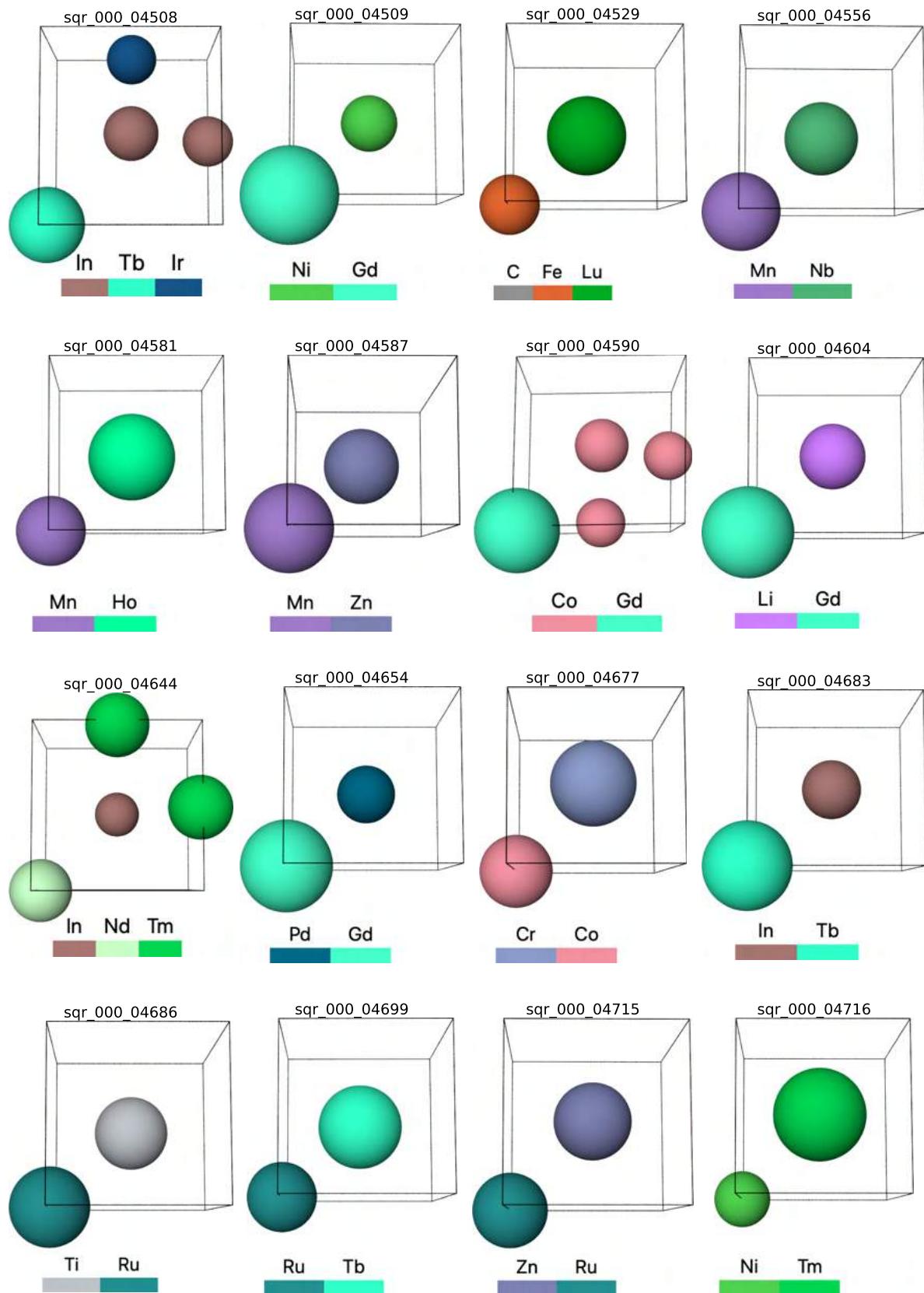


Figure S121. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

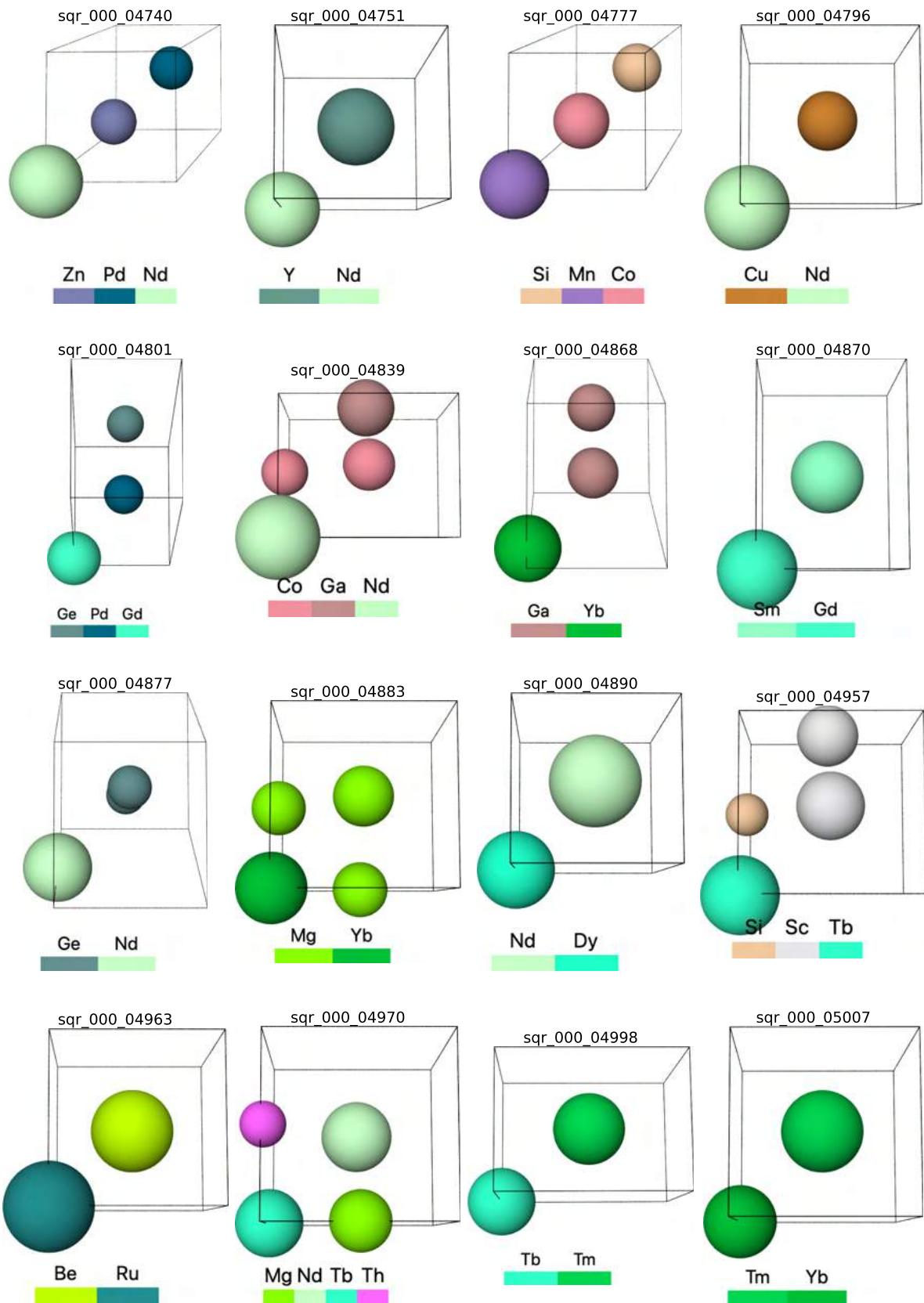


Figure S122. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

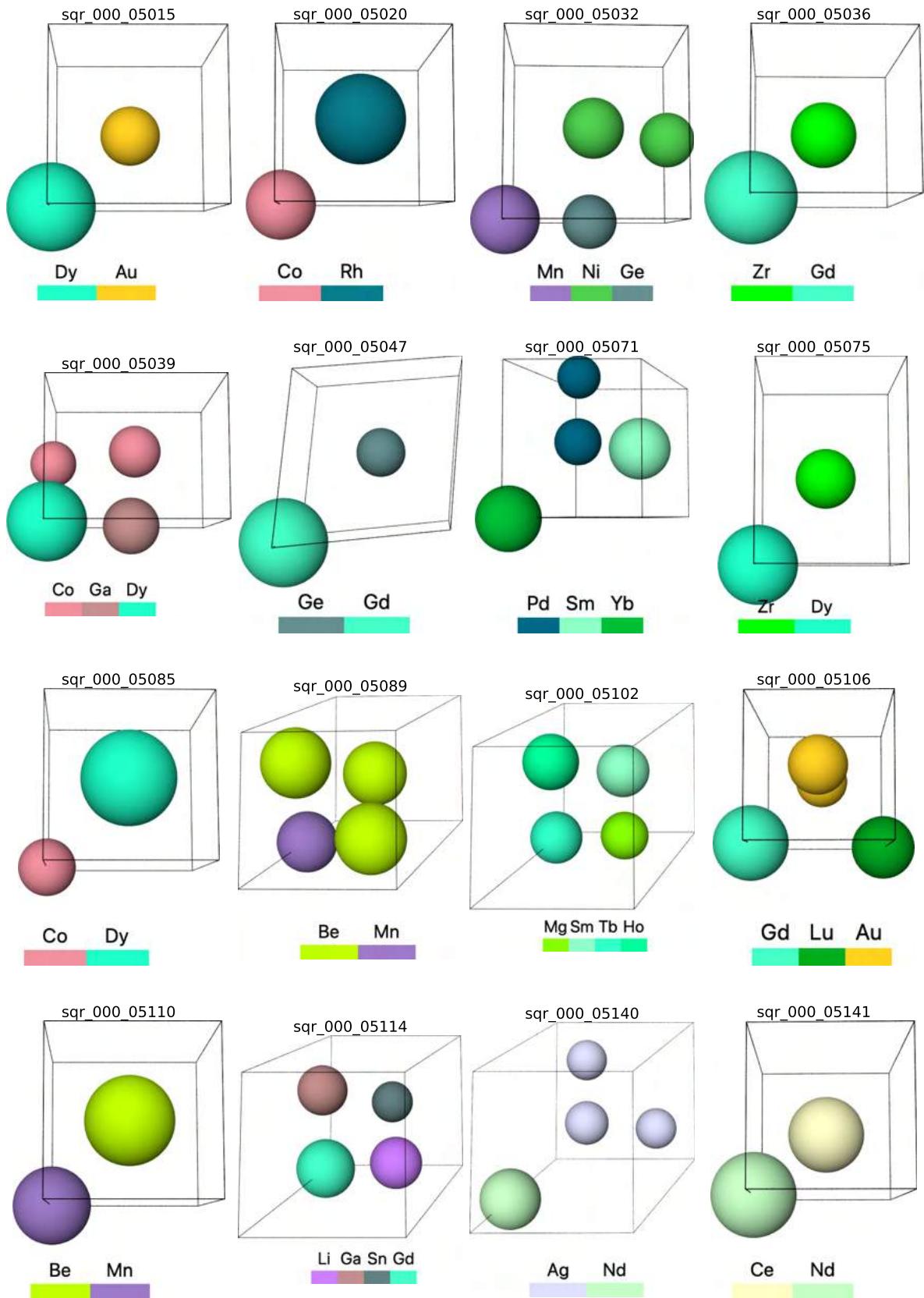


Figure S123. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

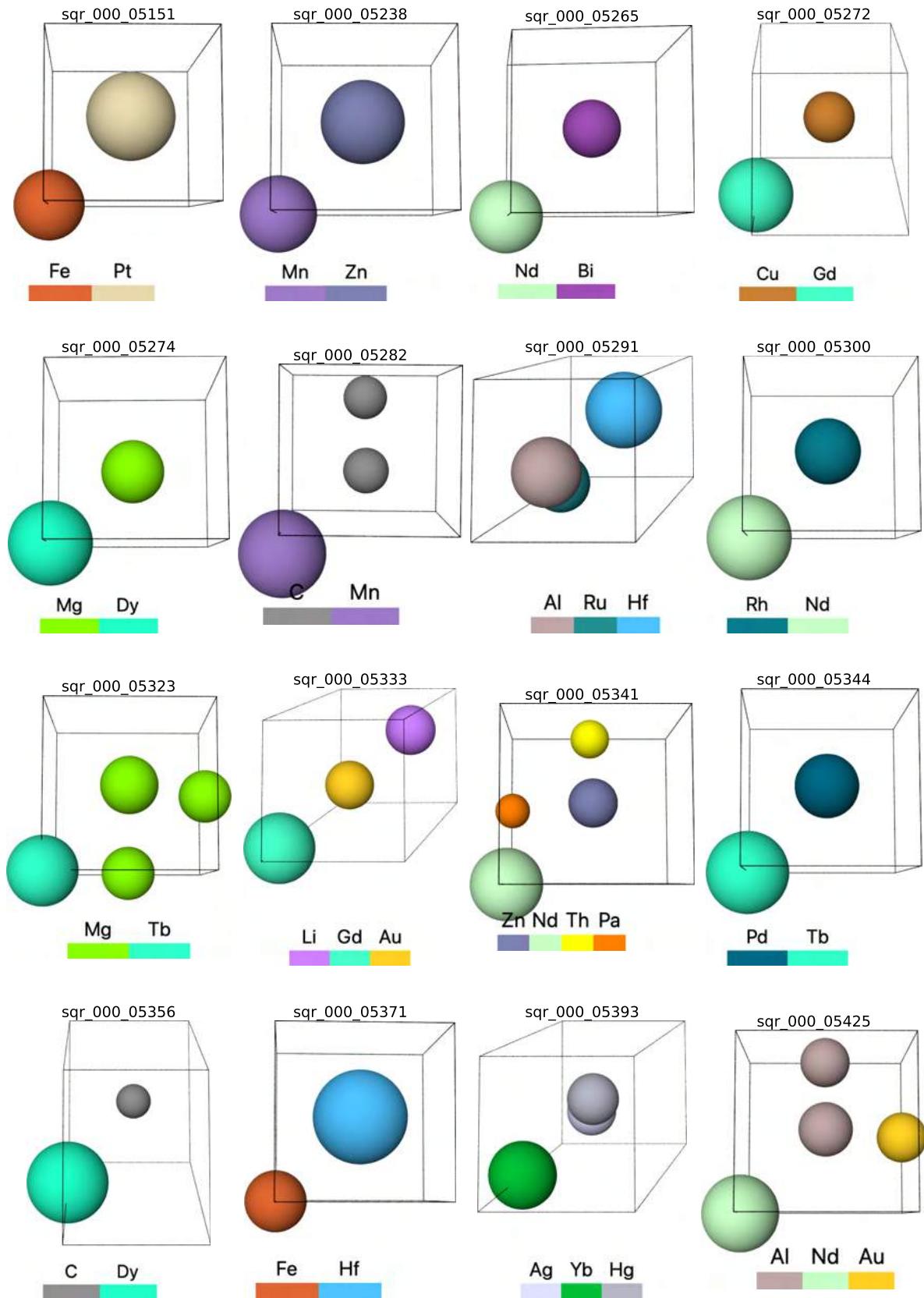


Figure S124. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

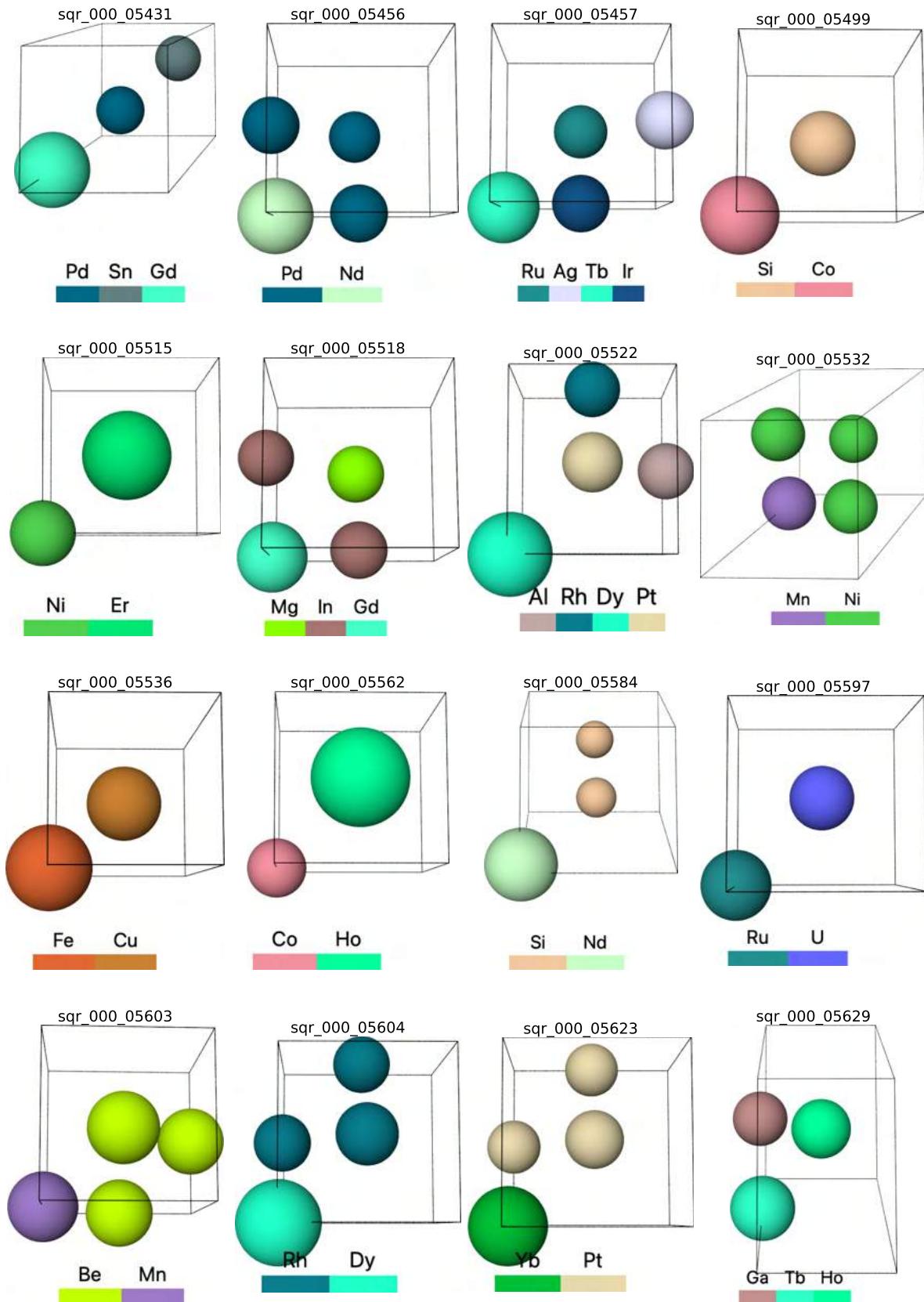


Figure S125. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

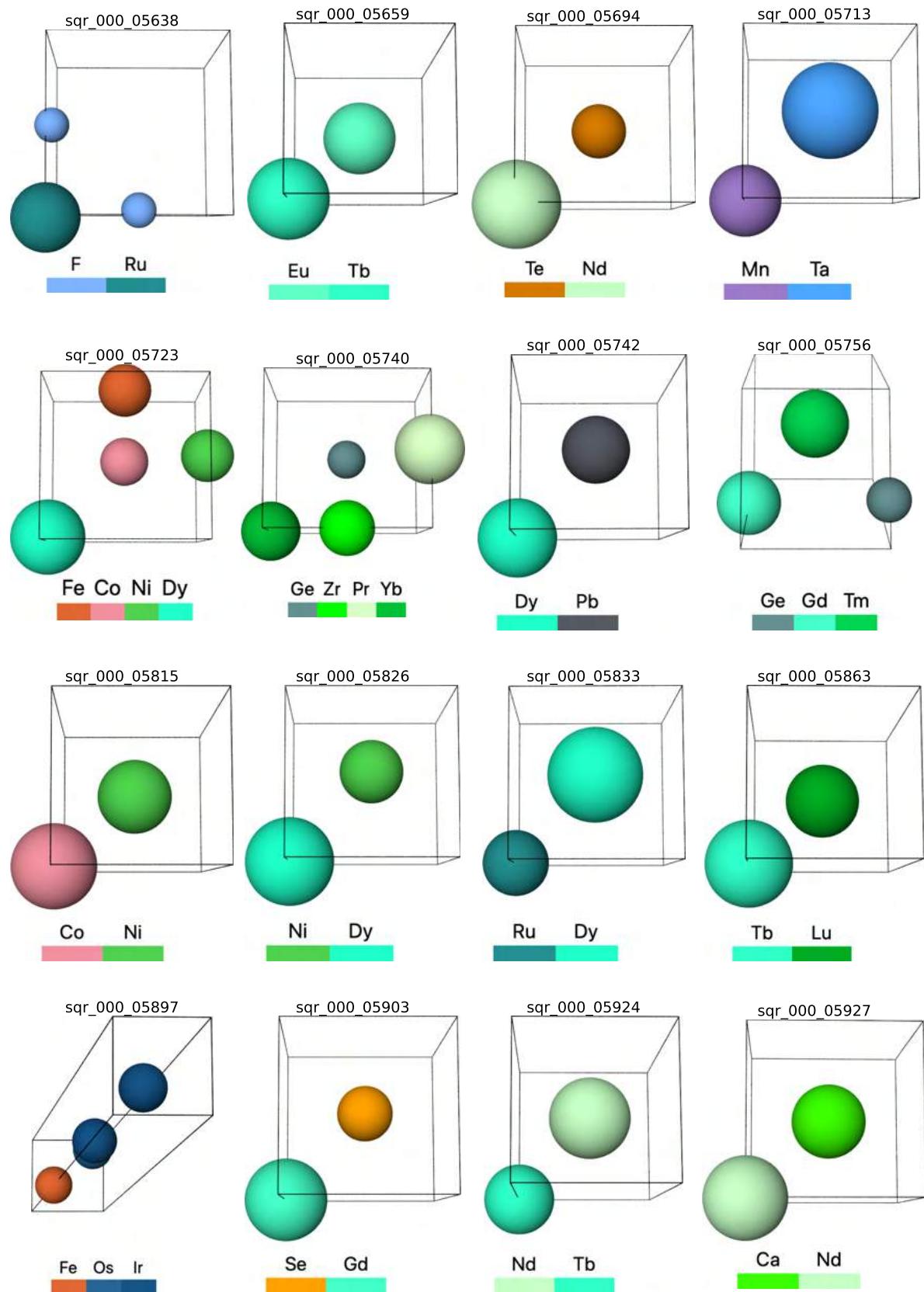


Figure S126. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

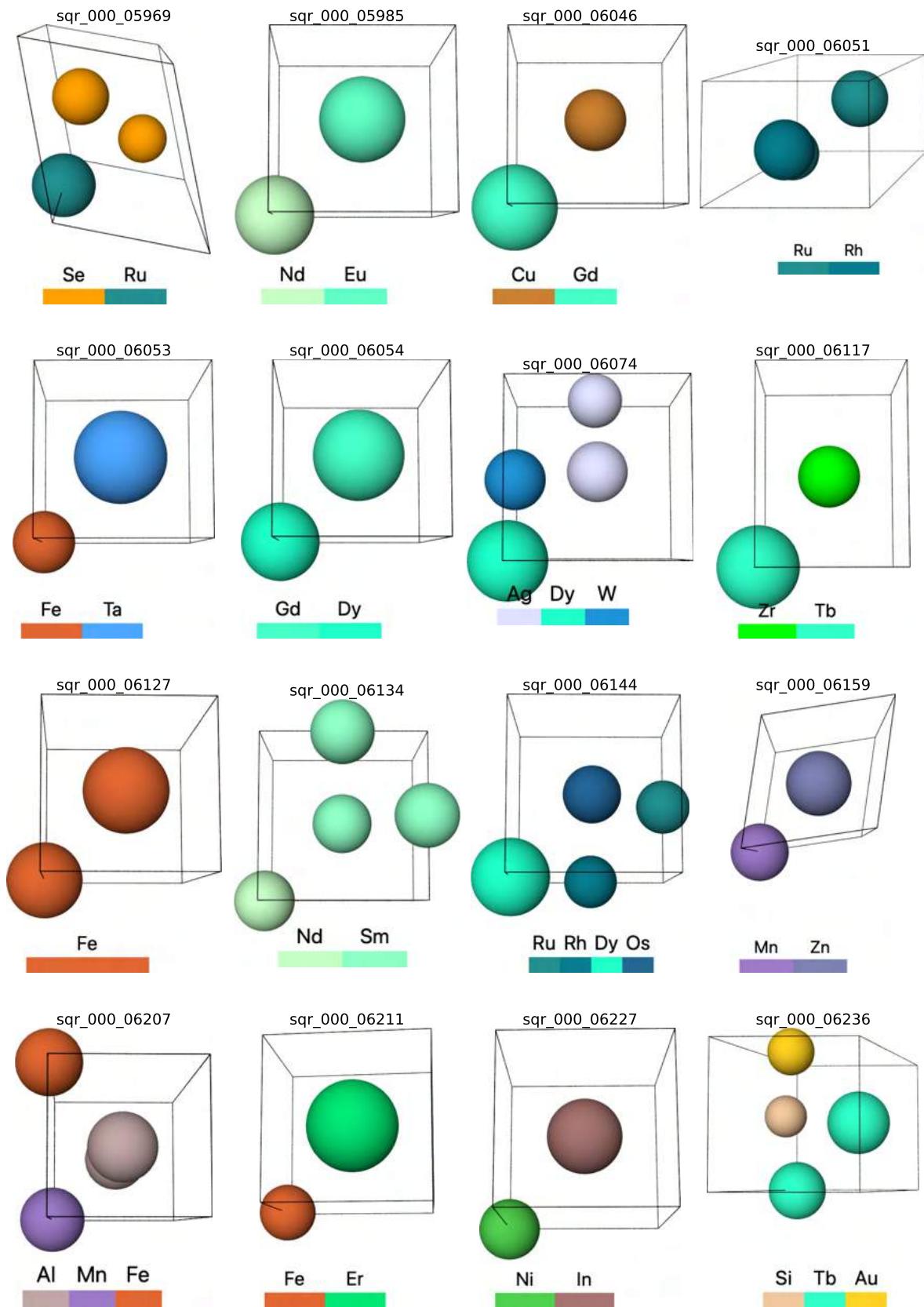


Figure S127. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

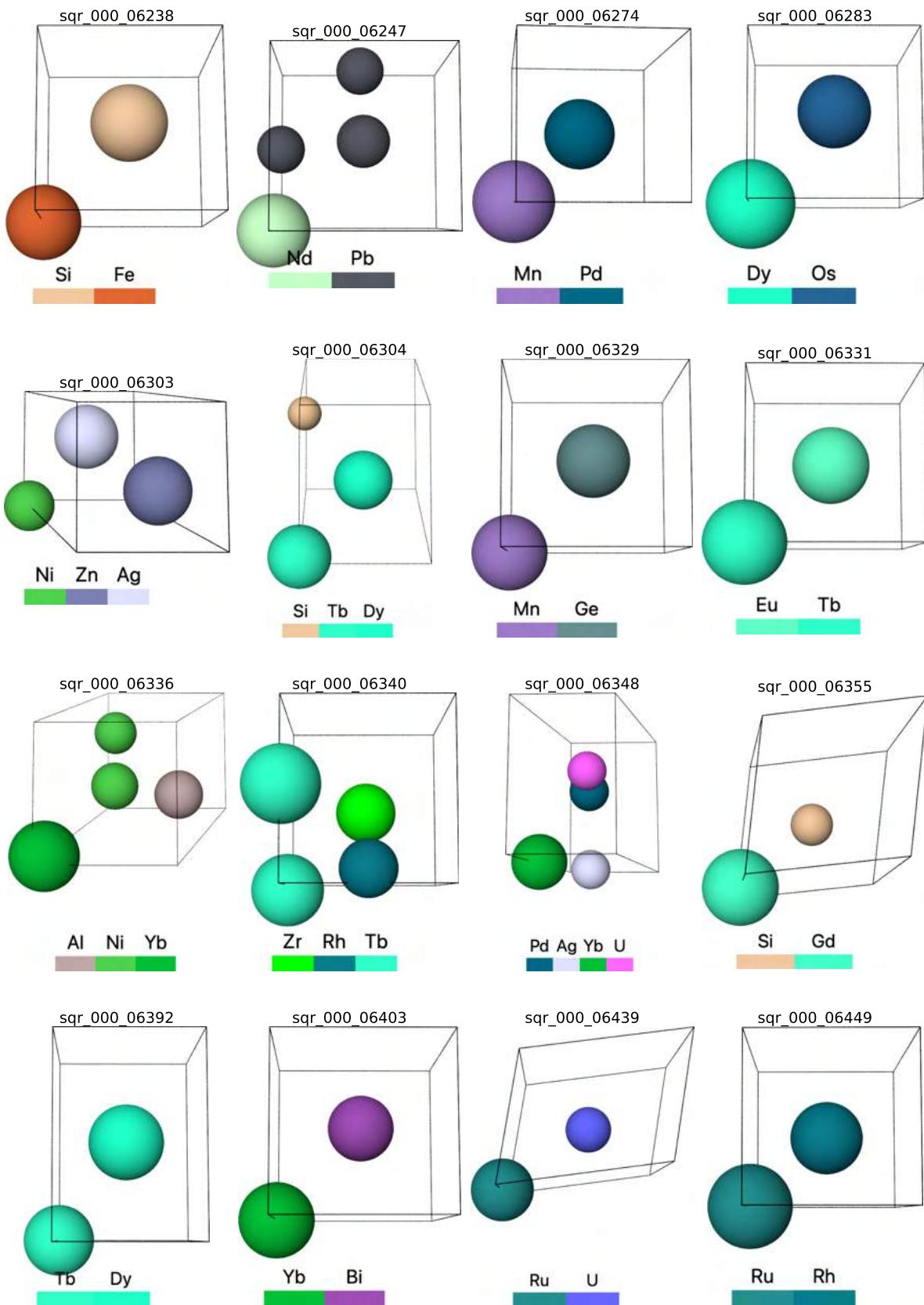


Figure S128. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

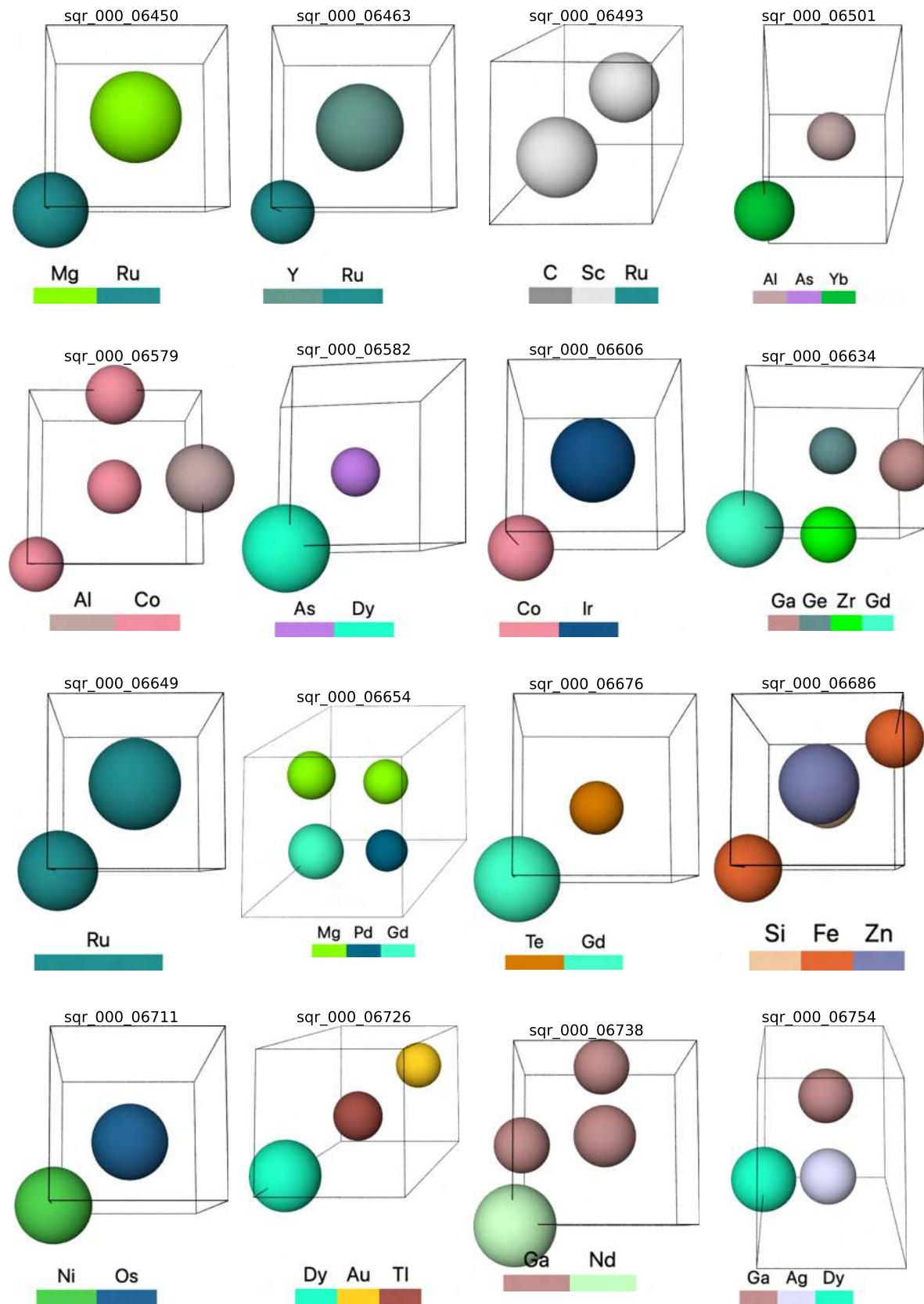


Figure S129. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

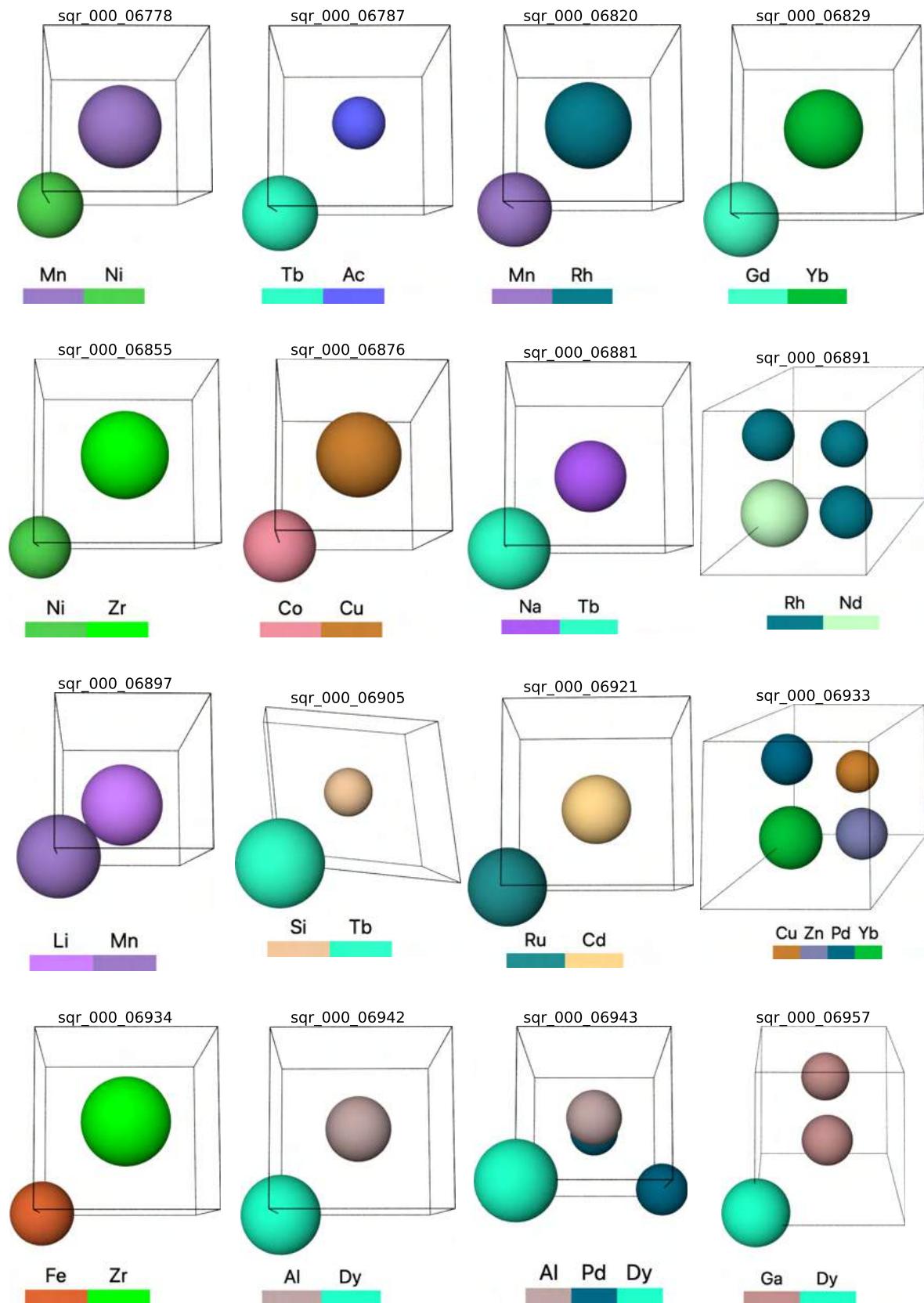


Figure S130. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

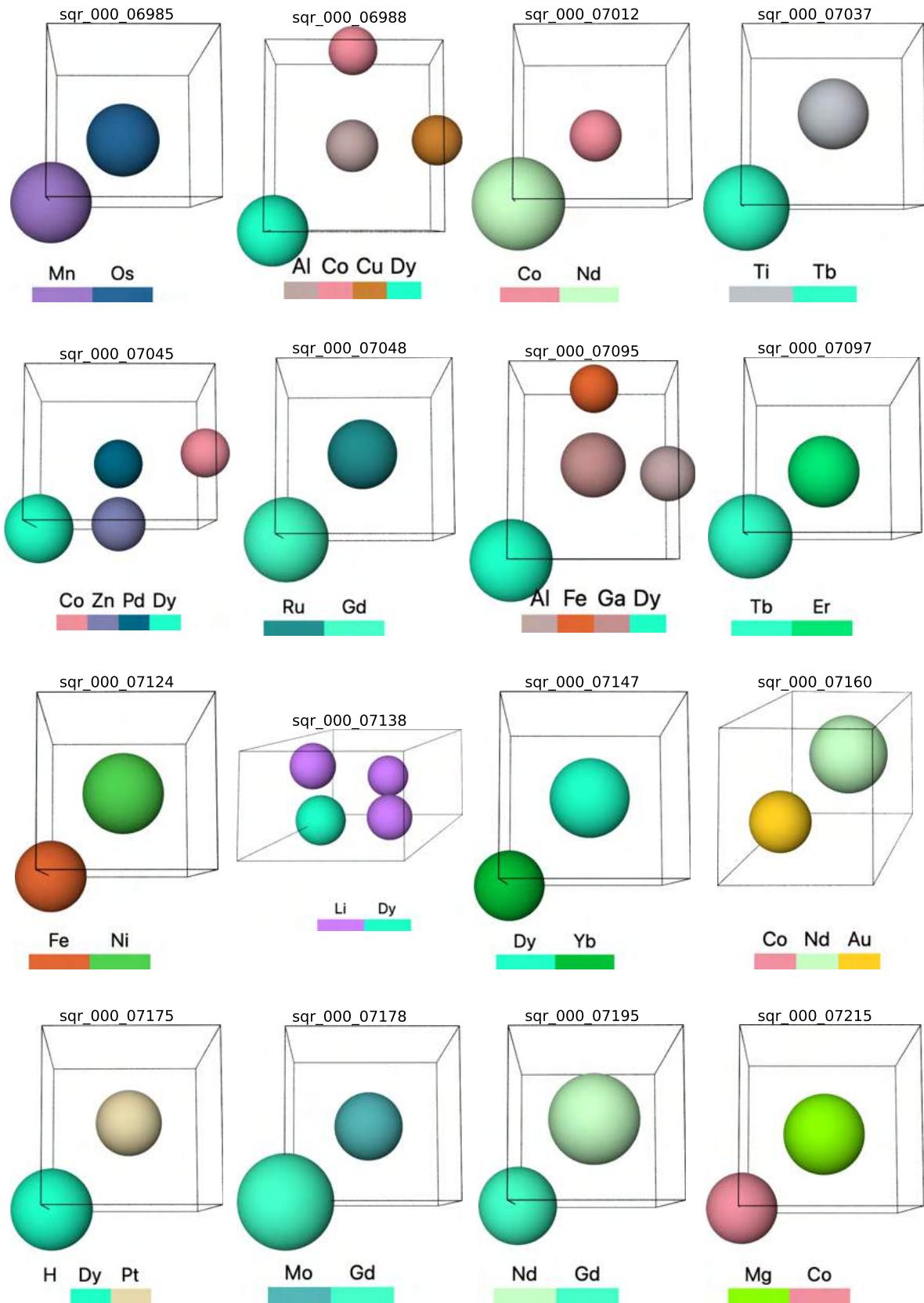


Figure S131. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

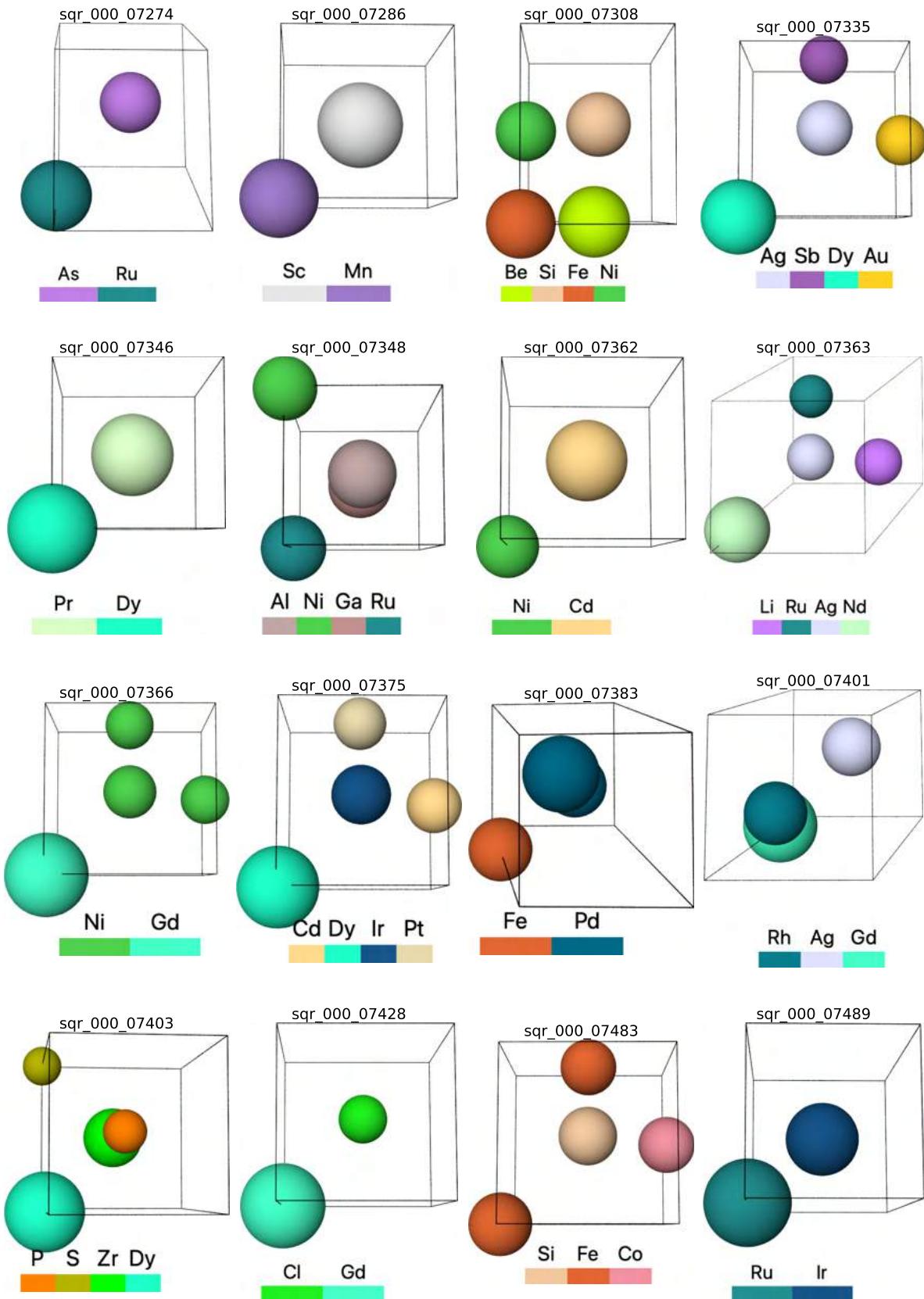


Figure S132. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

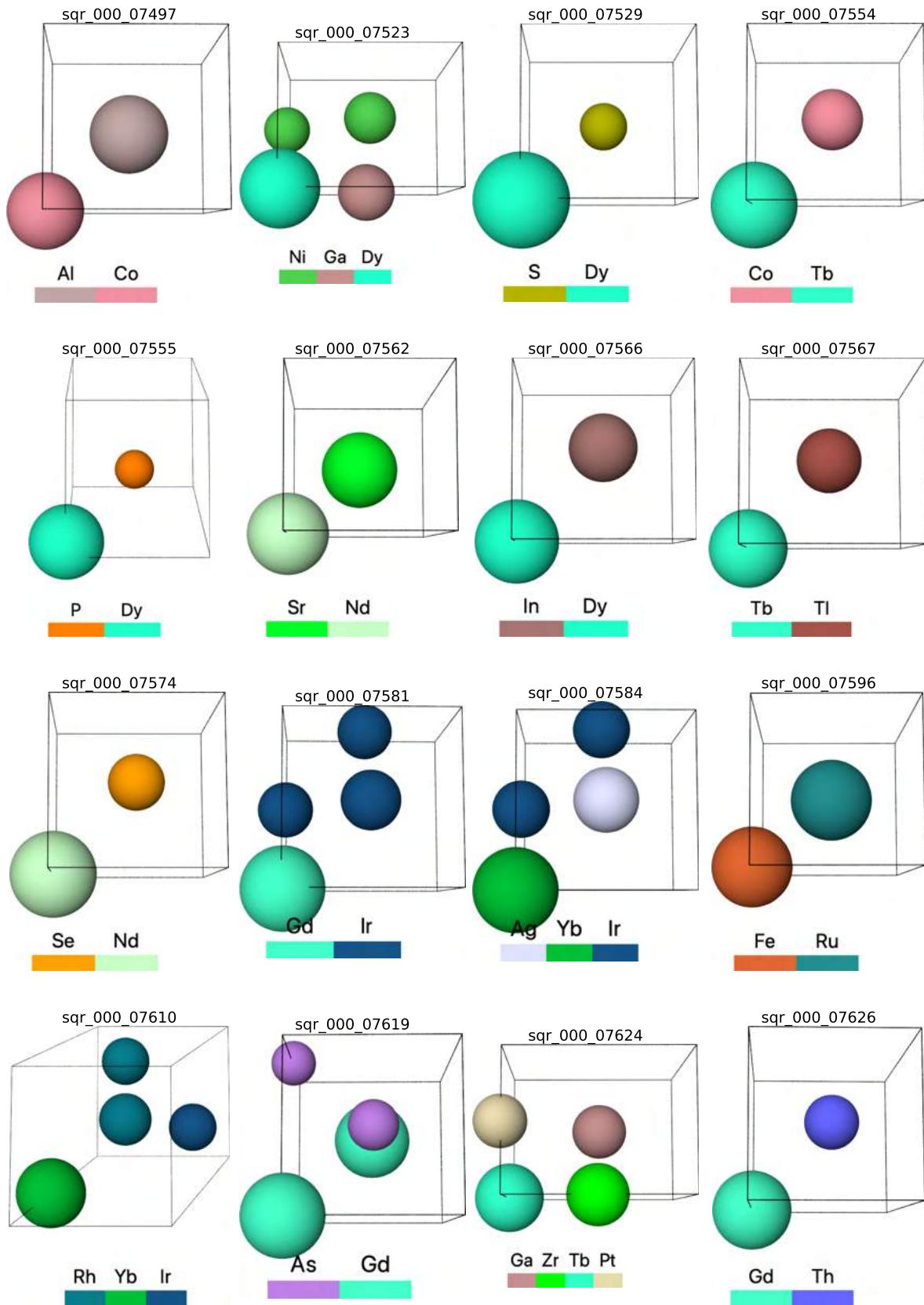


Figure S133. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

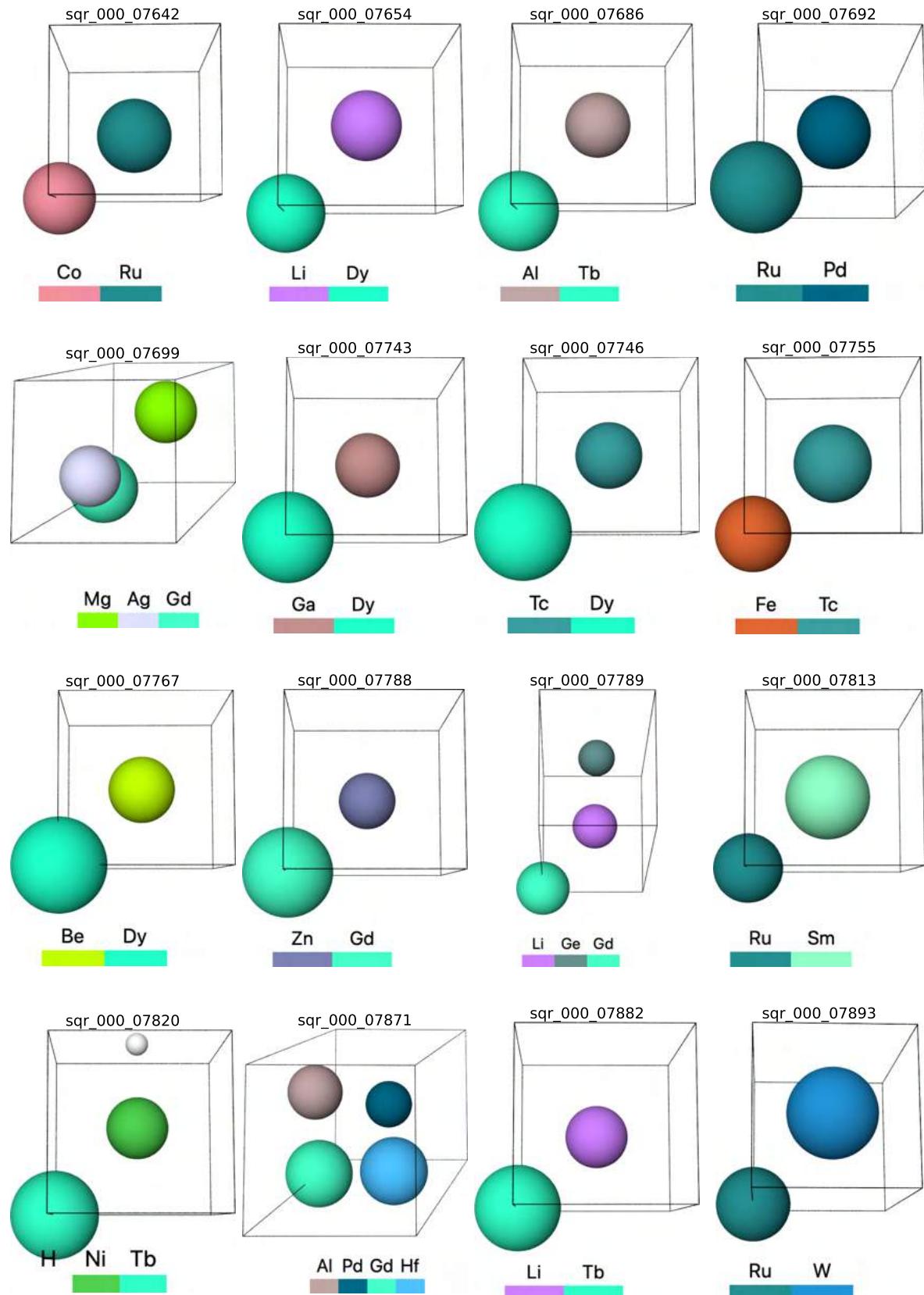


Figure S134. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

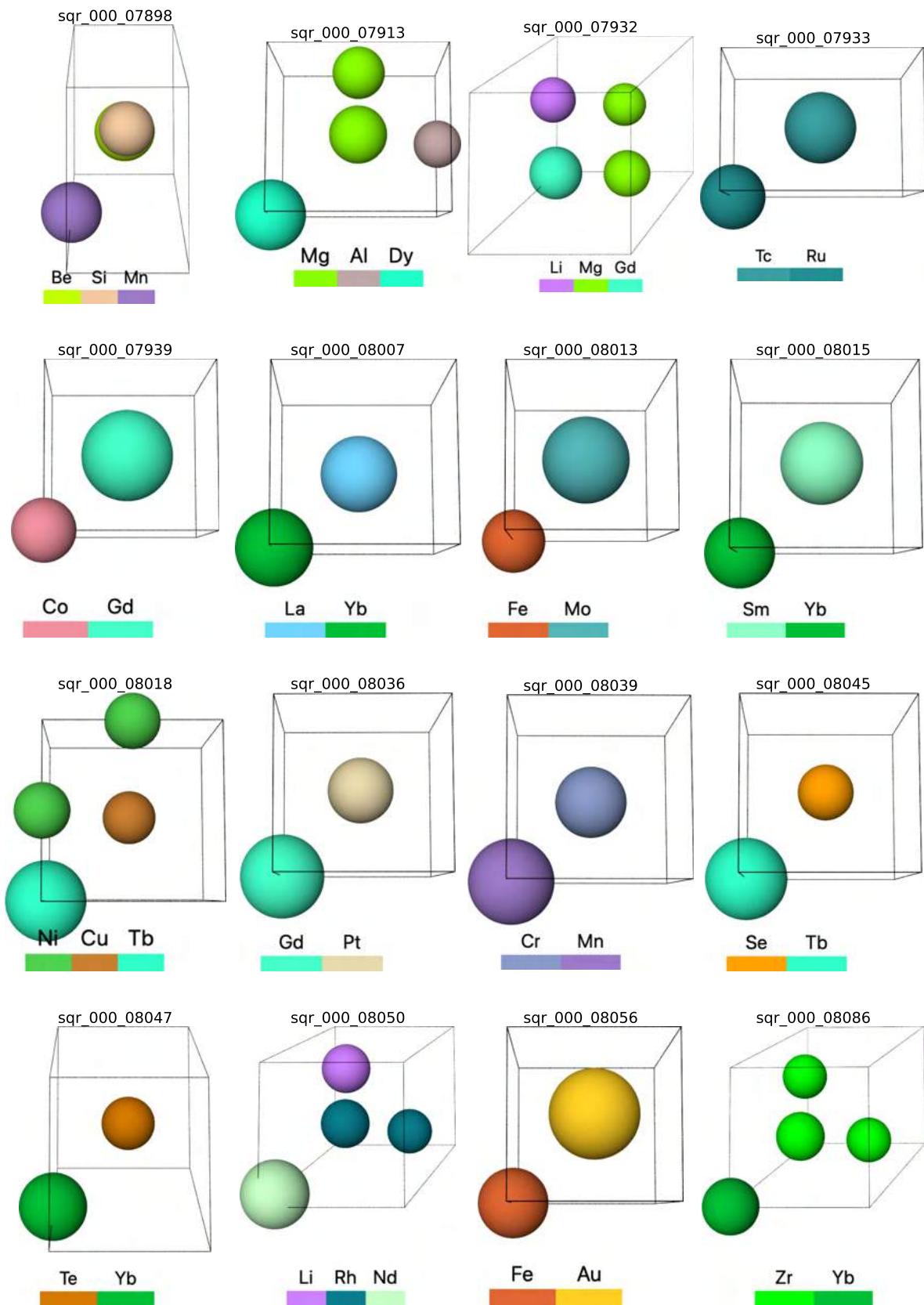


Figure S135. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

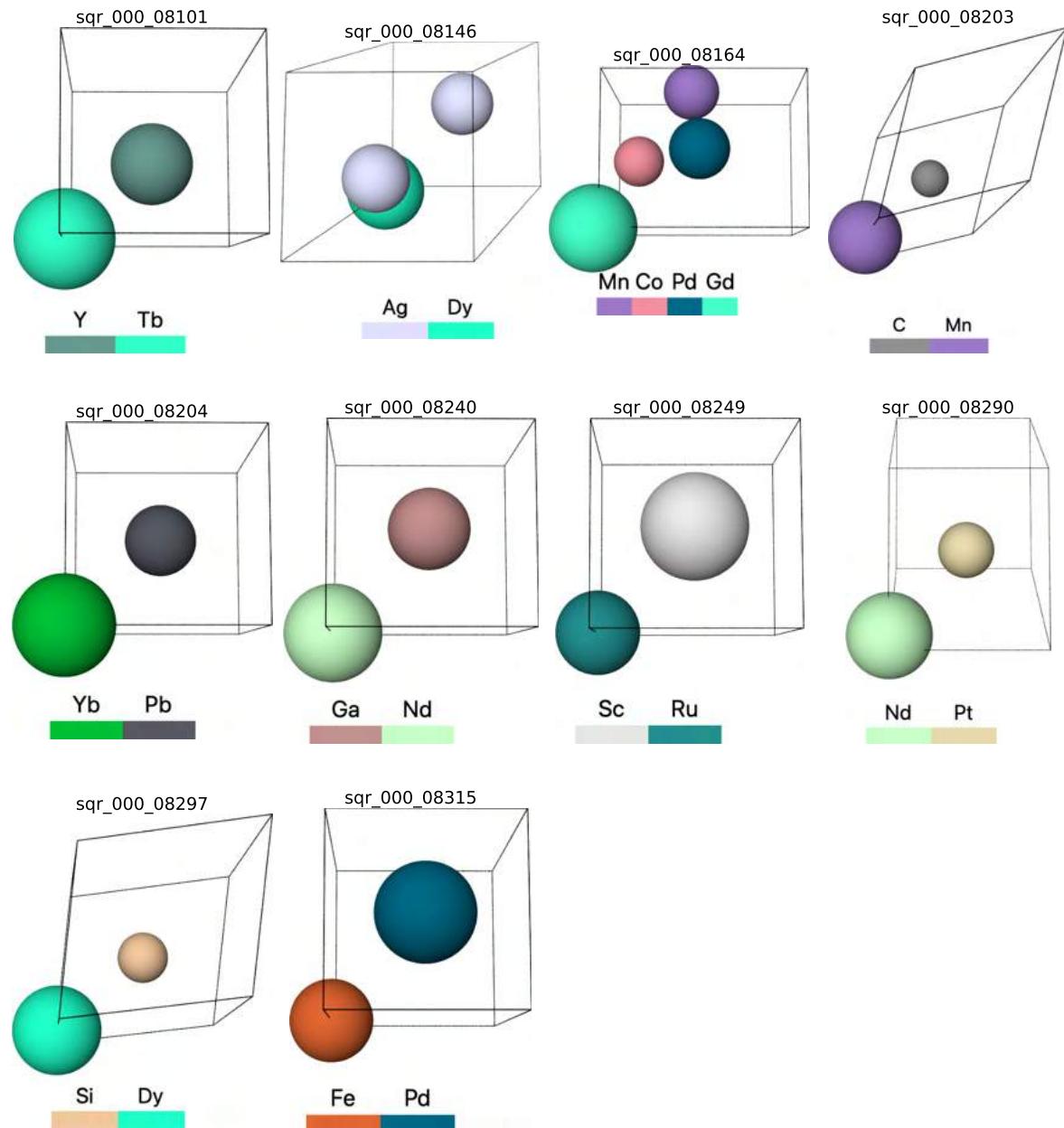


Figure S136. Generated materials with Square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

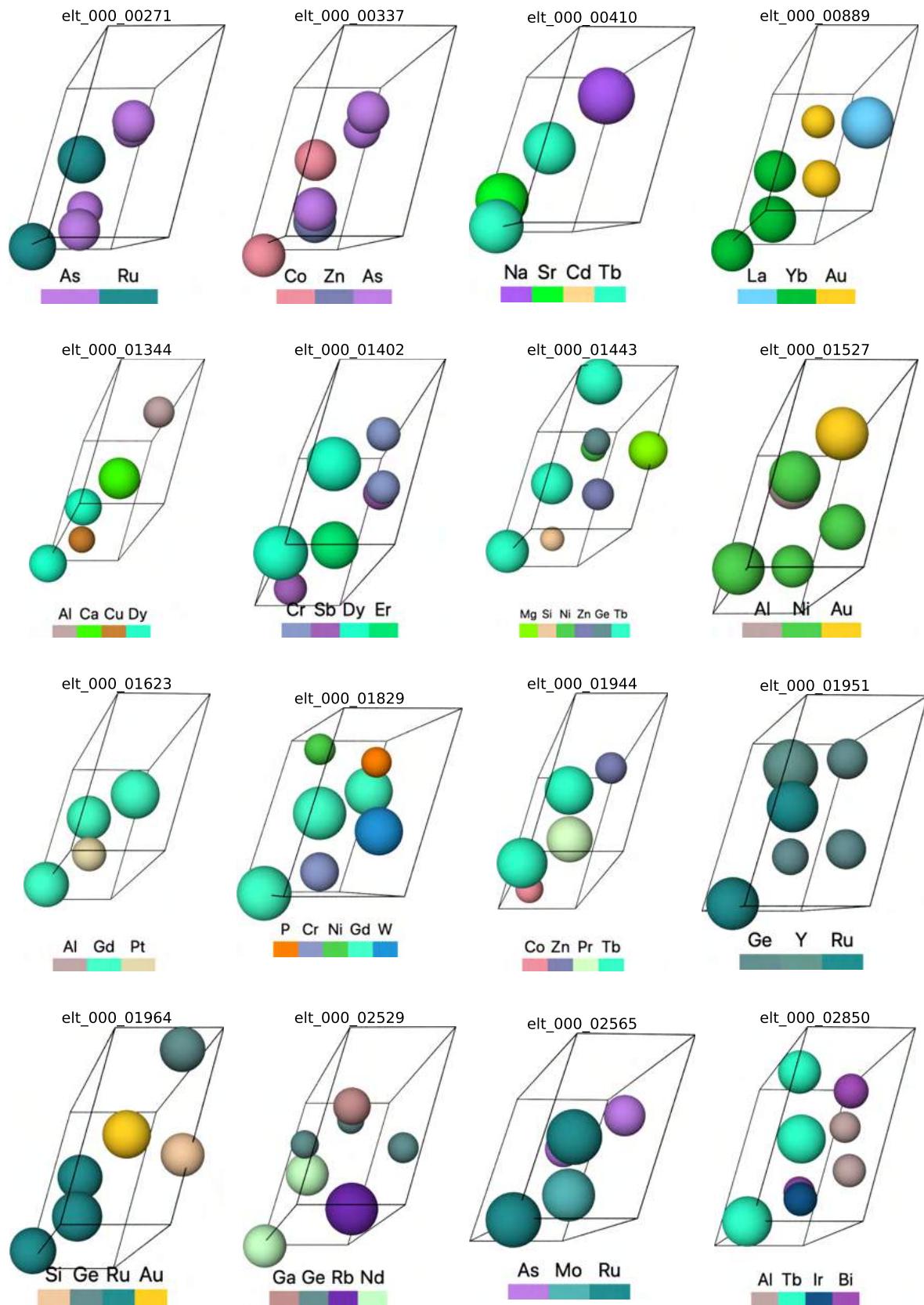


Figure S137. Generated materials with Elongated triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

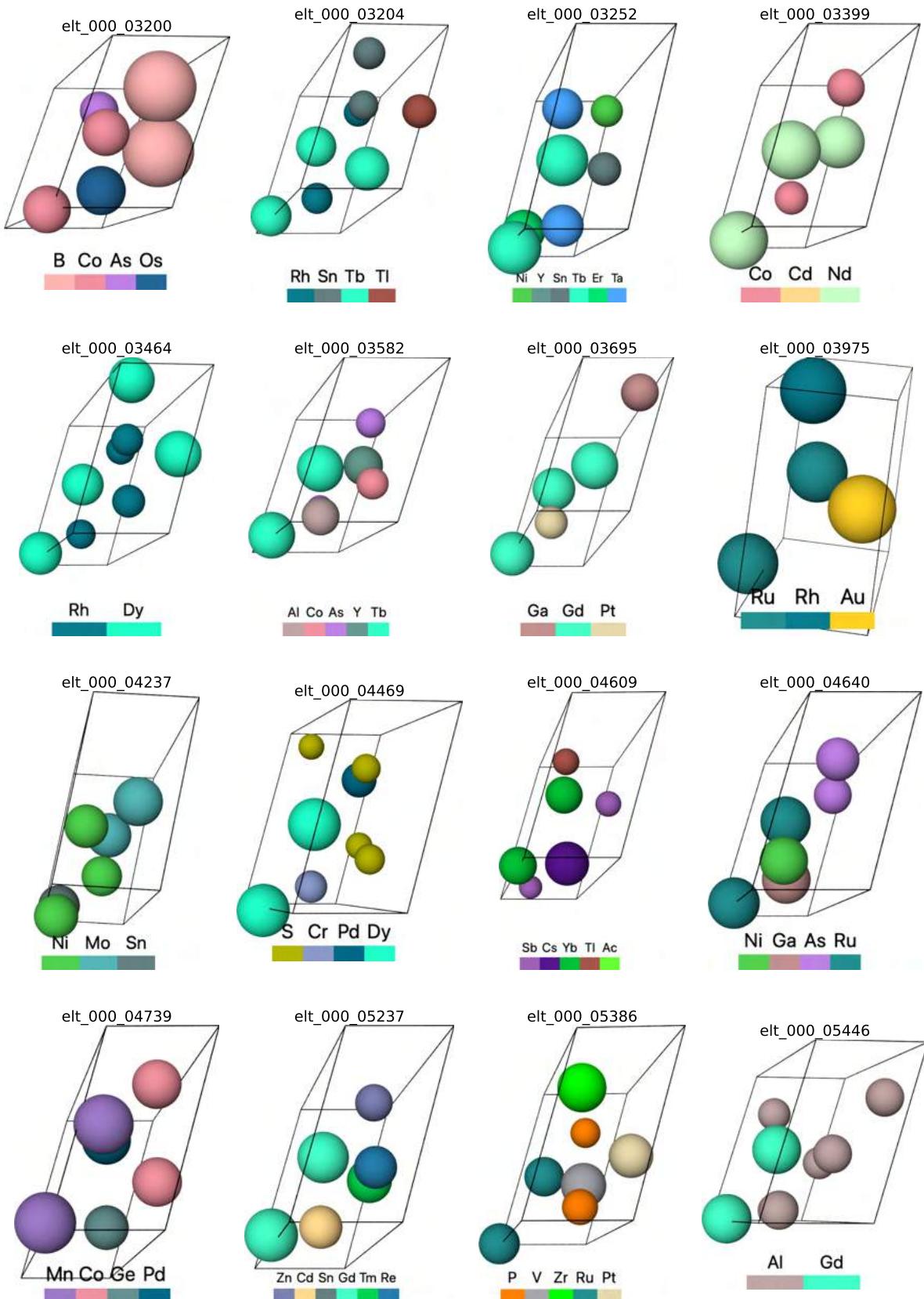


Figure S138. Generated materials with Elongated triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

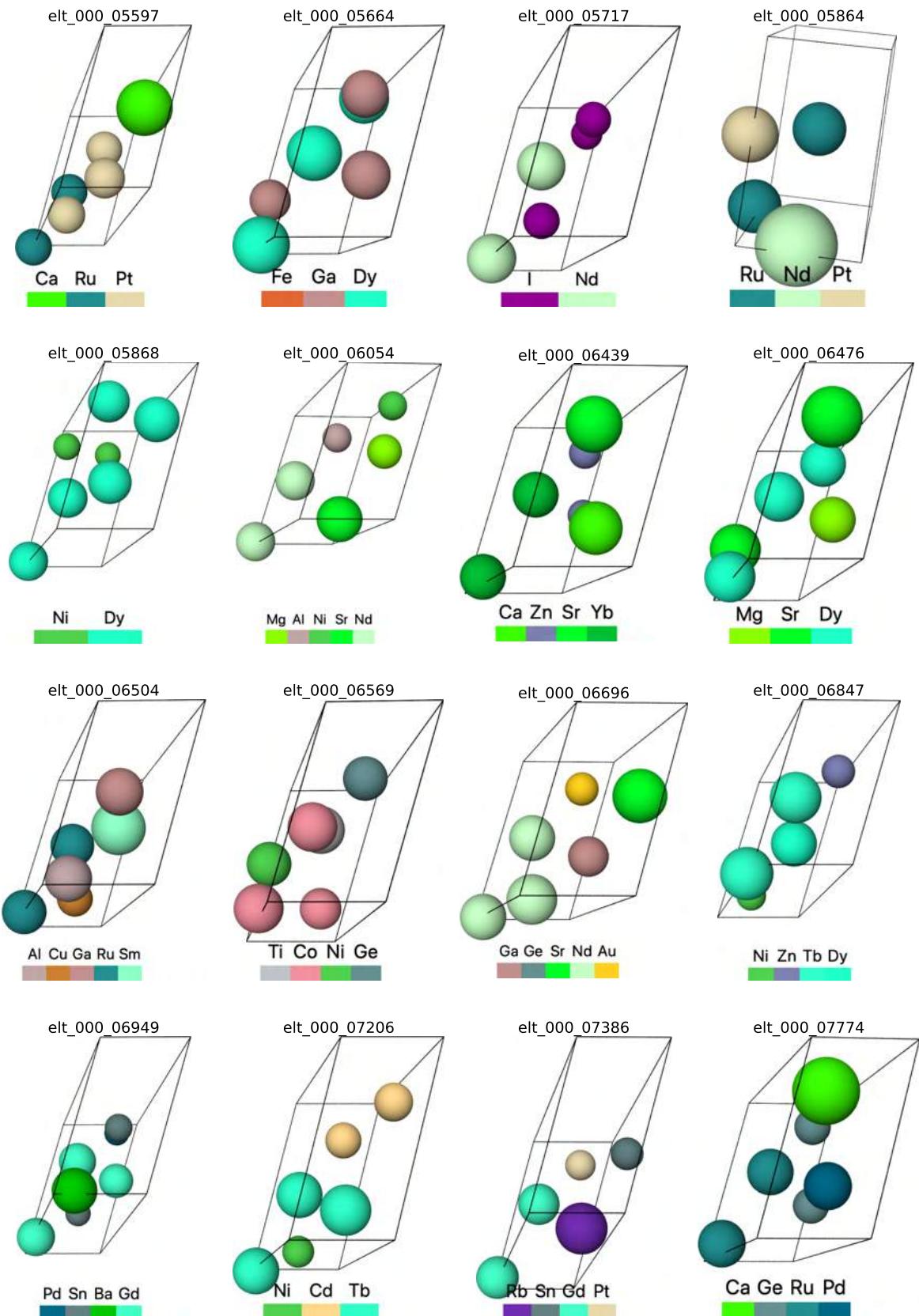


Figure S139. Generated materials with Elongated triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

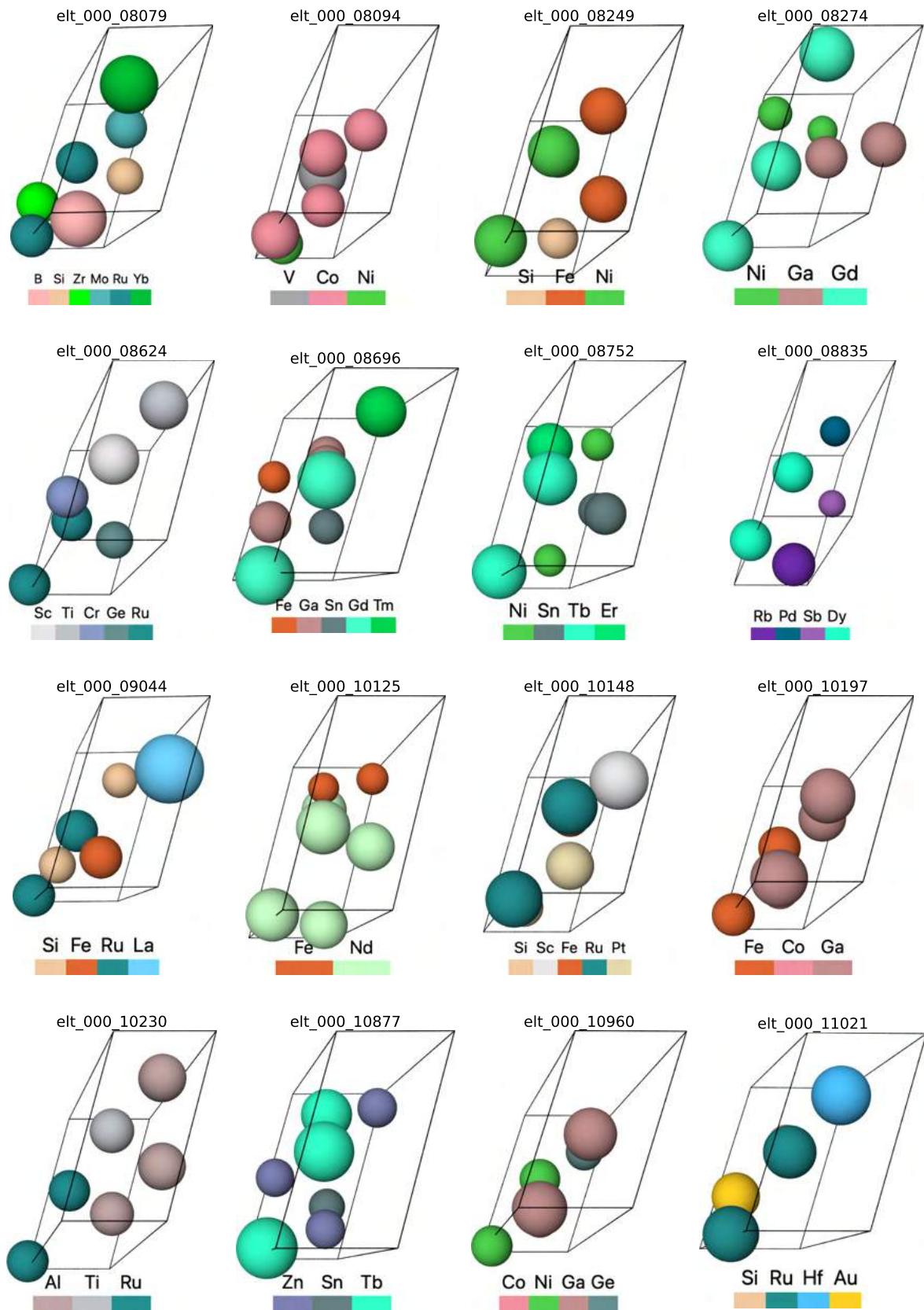


Figure S140. Generated materials with Elongated triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

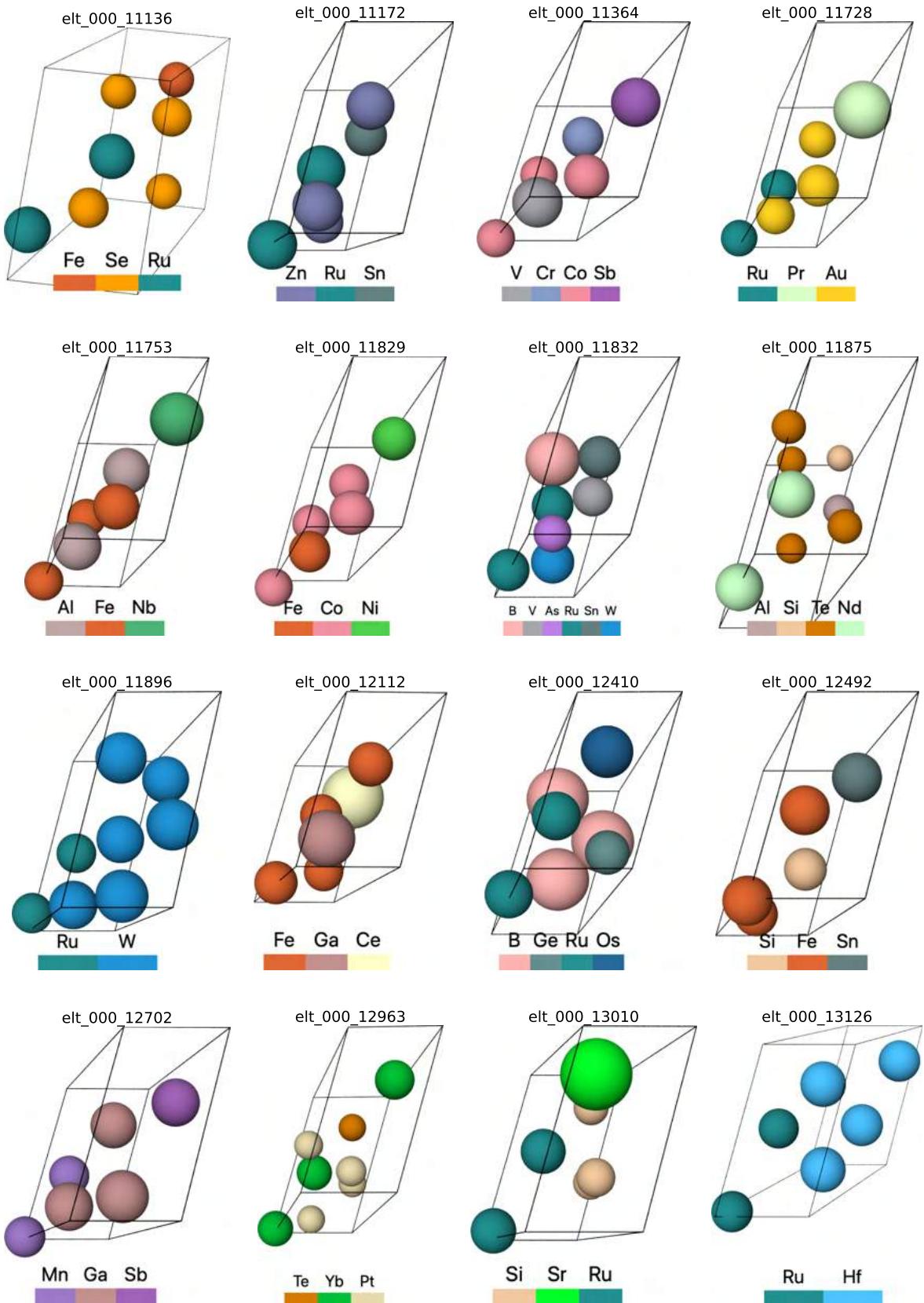


Figure S141. Generated materials with Elongated triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

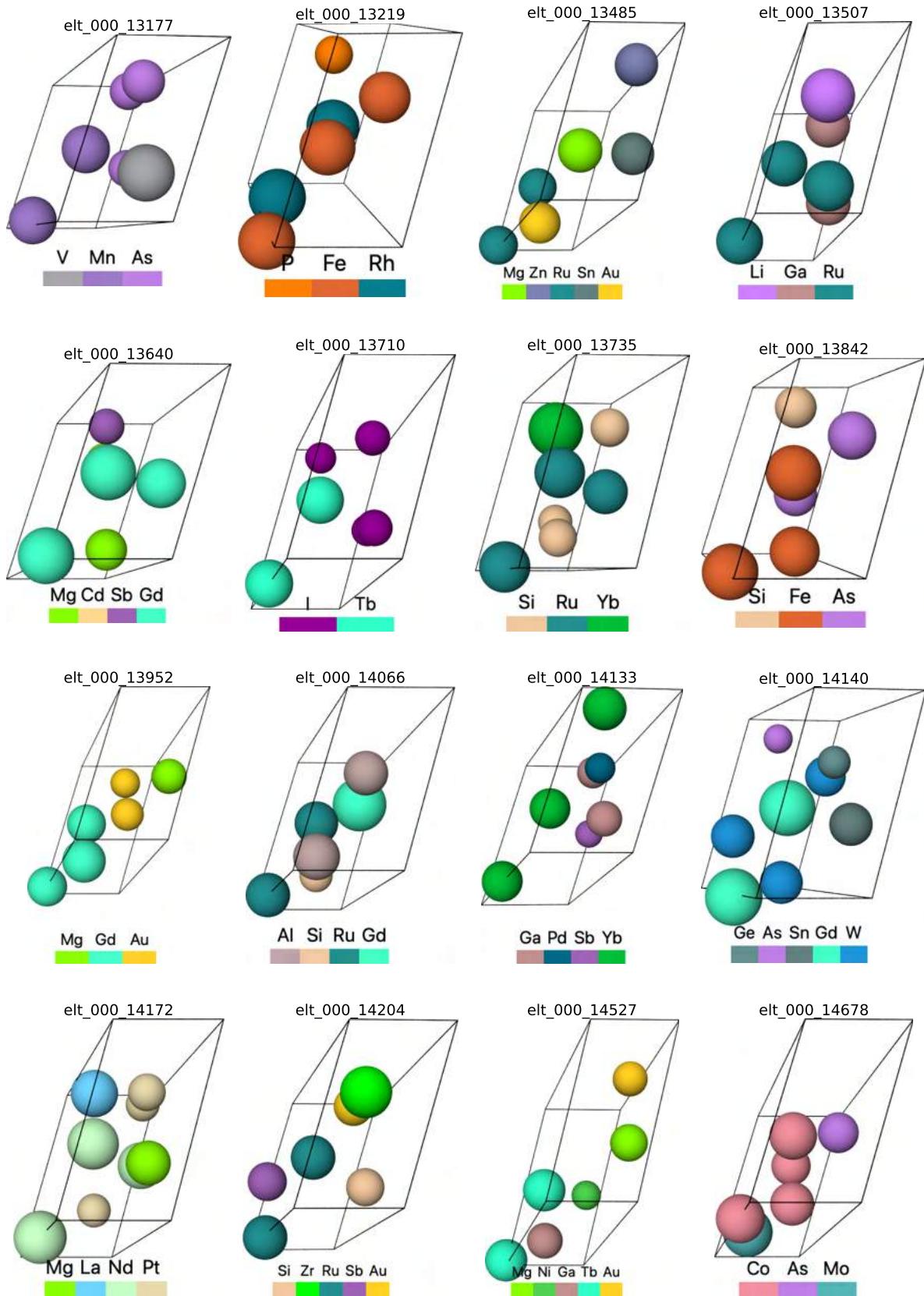


Figure S142. Generated materials with Elongated triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

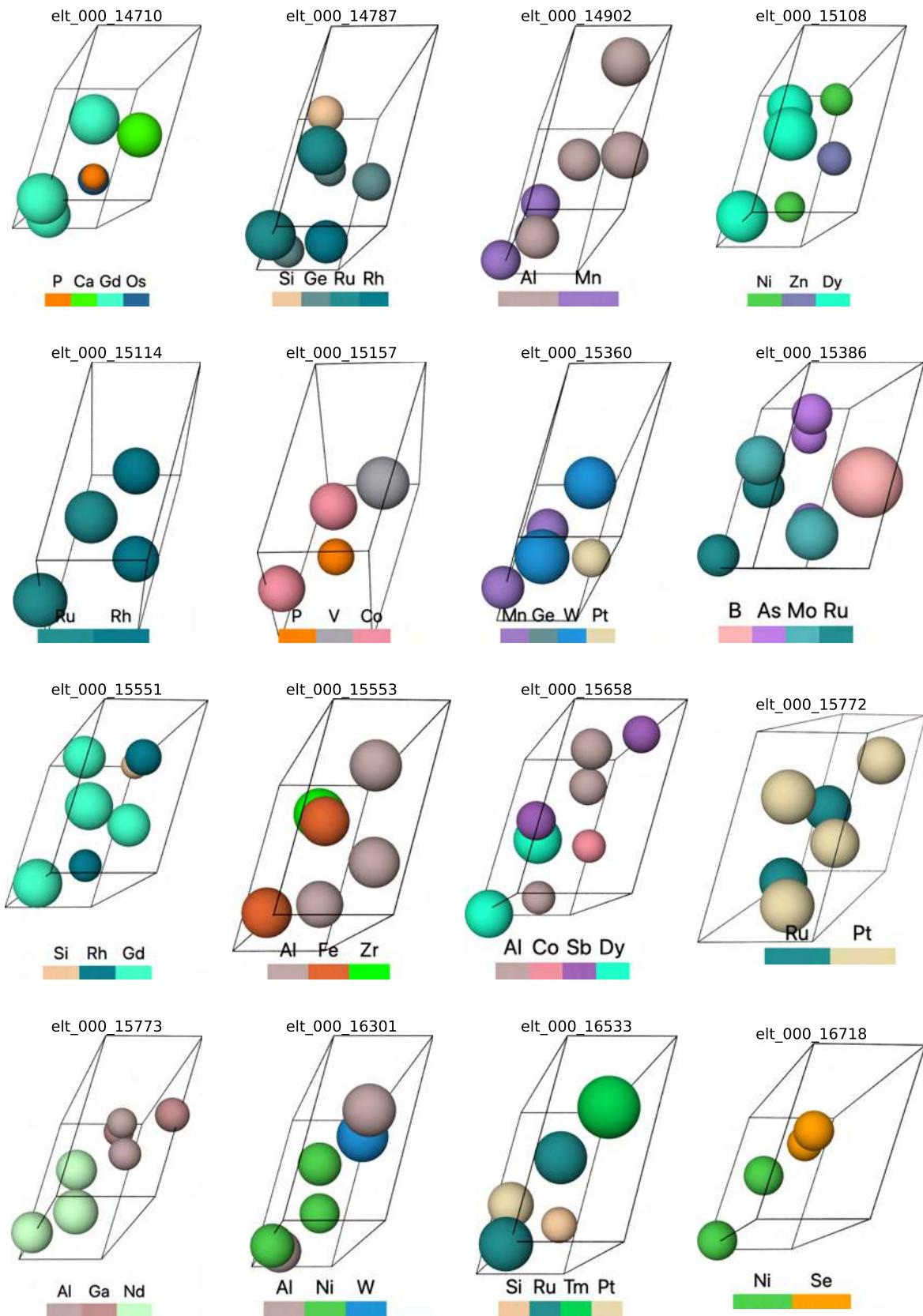


Figure S143. Generated materials with Elongated triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

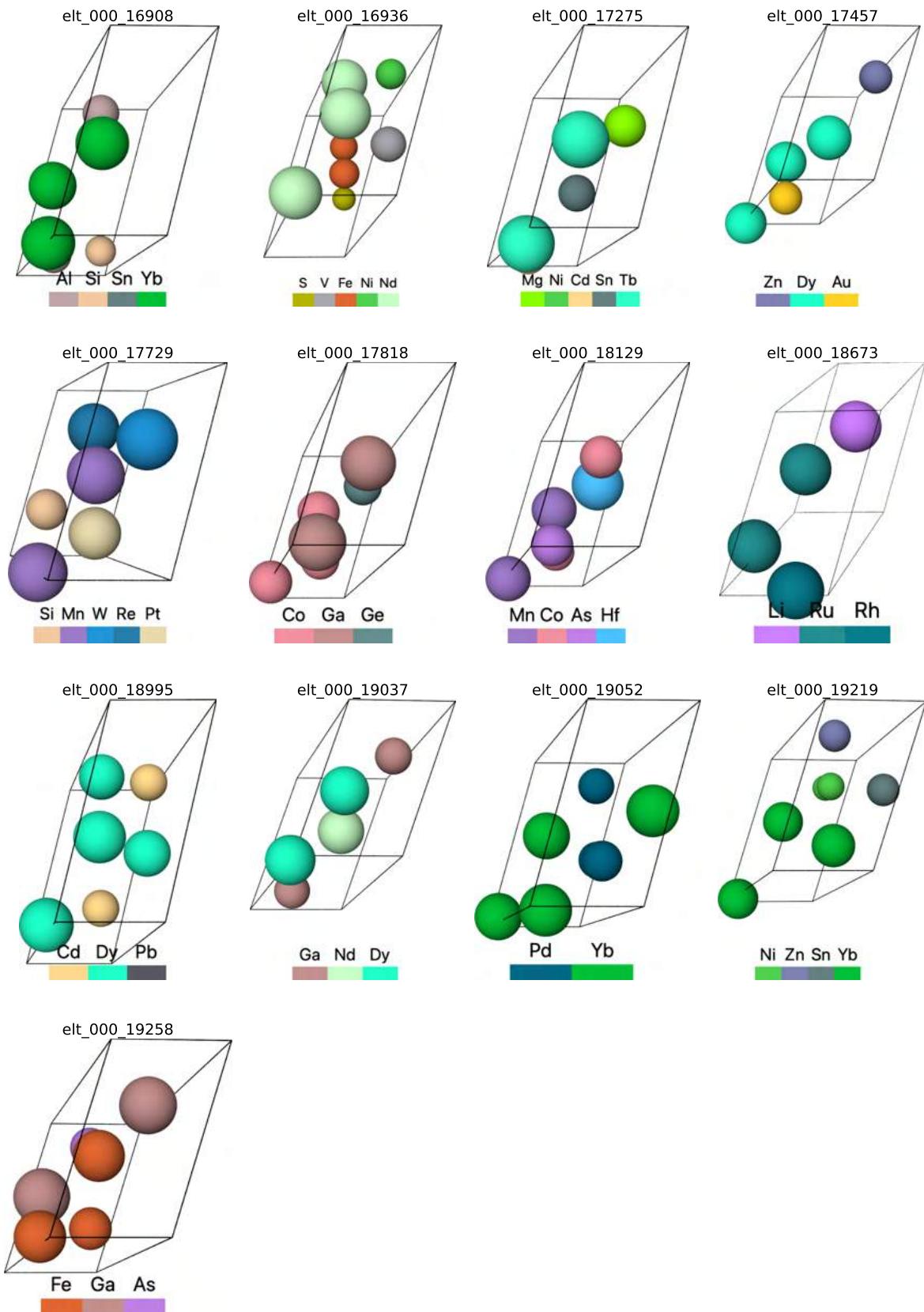


Figure S144. Generated materials with Elongated triangular lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

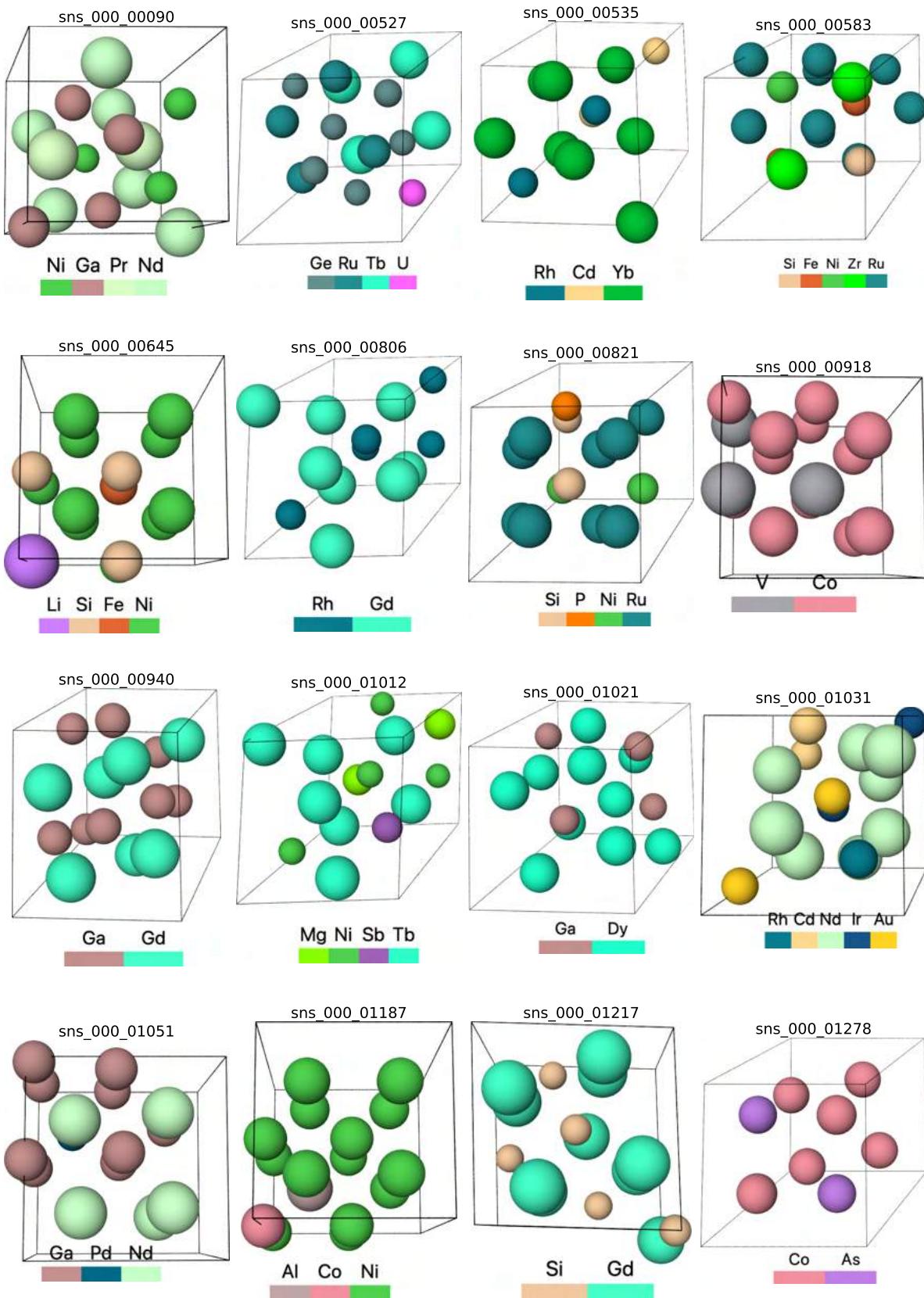


Figure S145. Generated materials with Snub square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

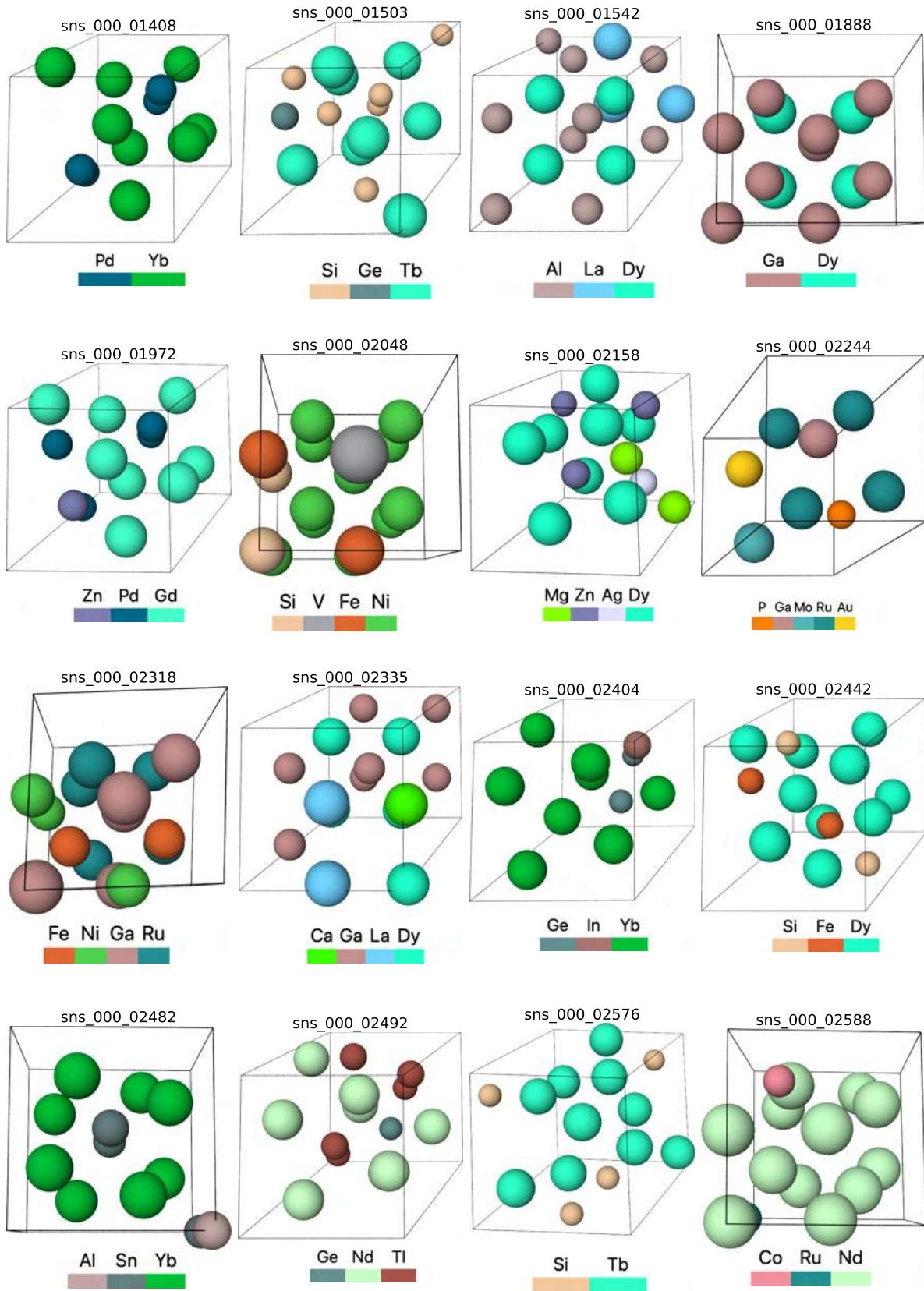


Figure S146. Generated materials with Snub square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

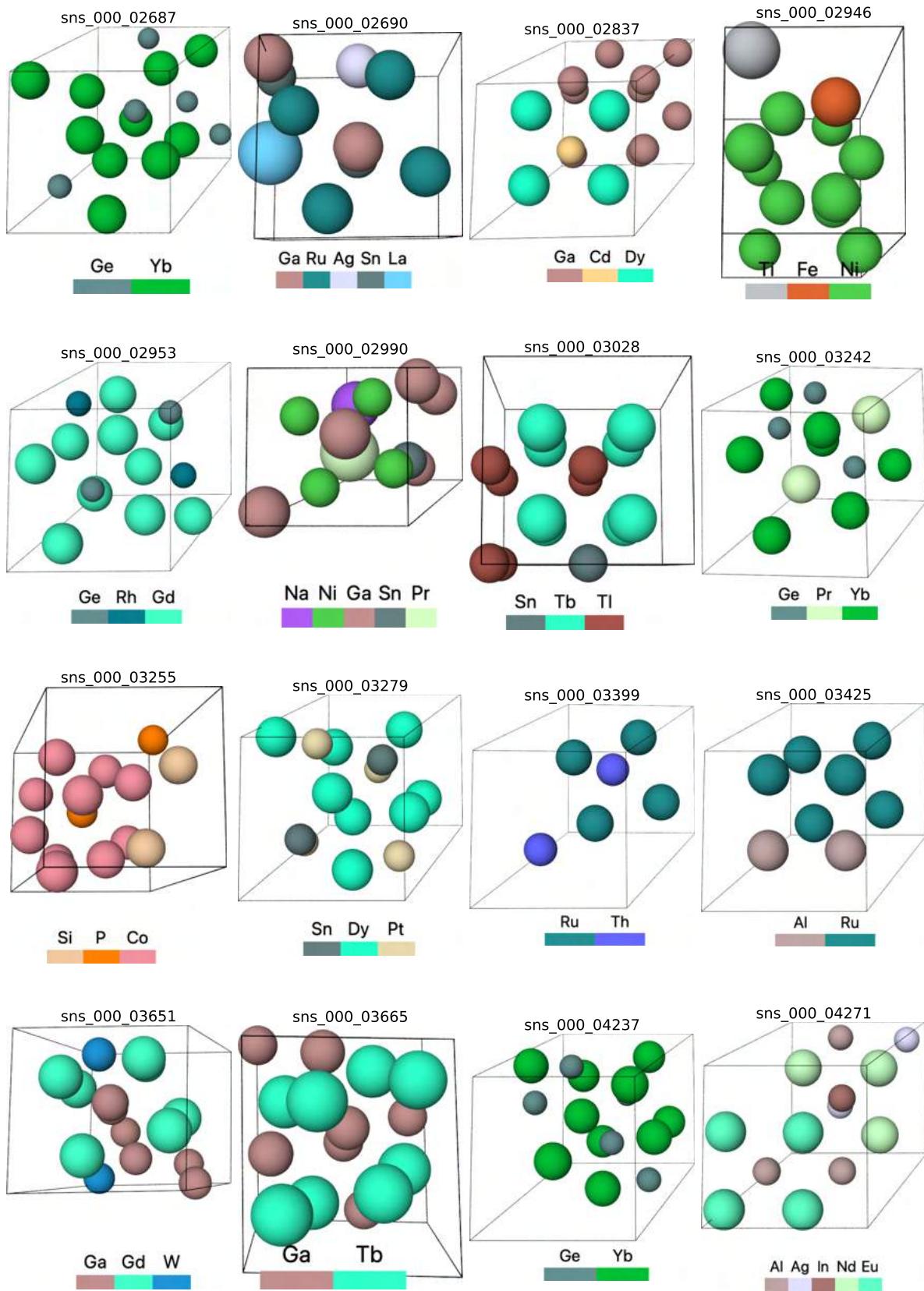


Figure S147. Generated materials with Snub square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

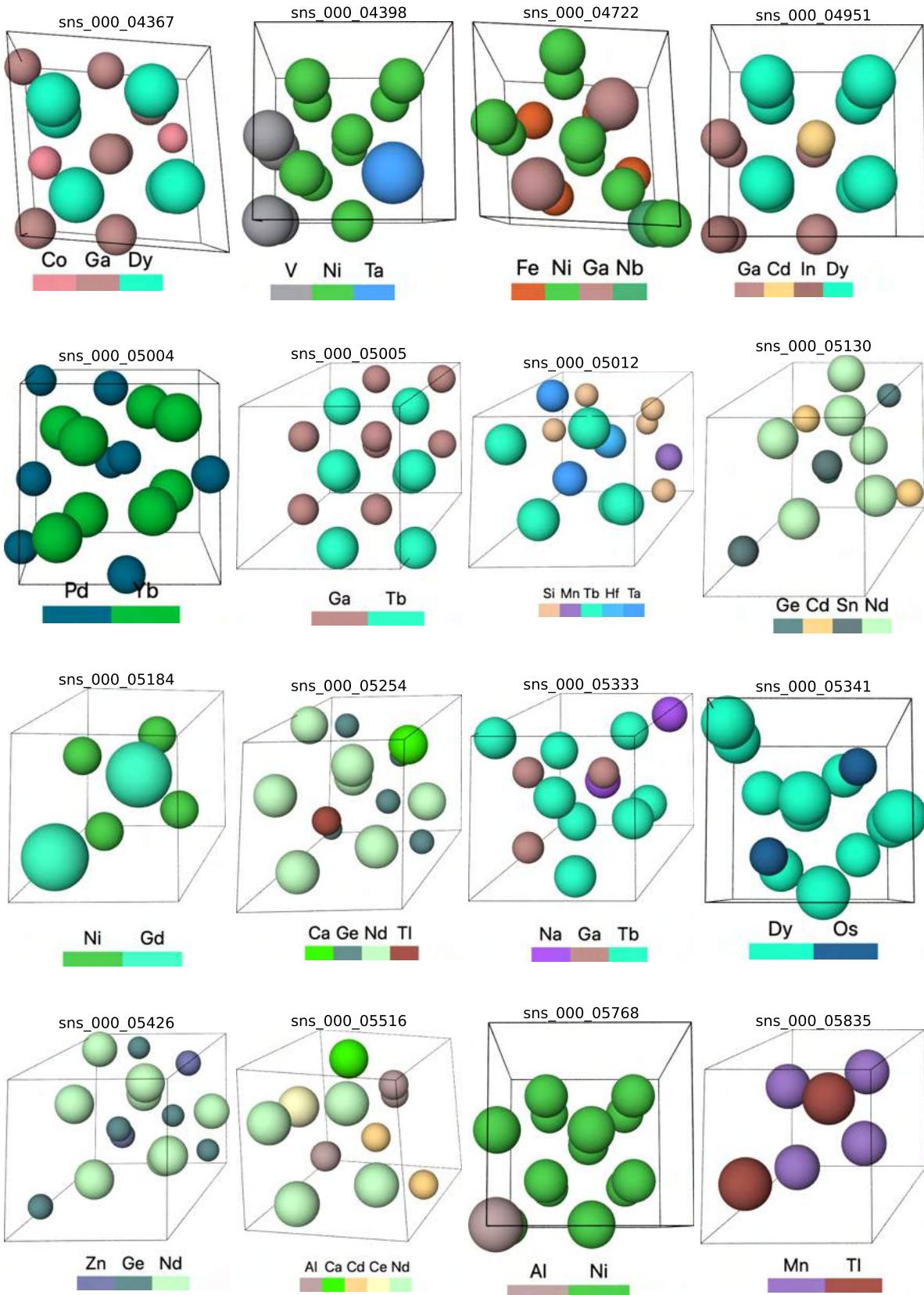


Figure S148. Generated materials with Snub square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

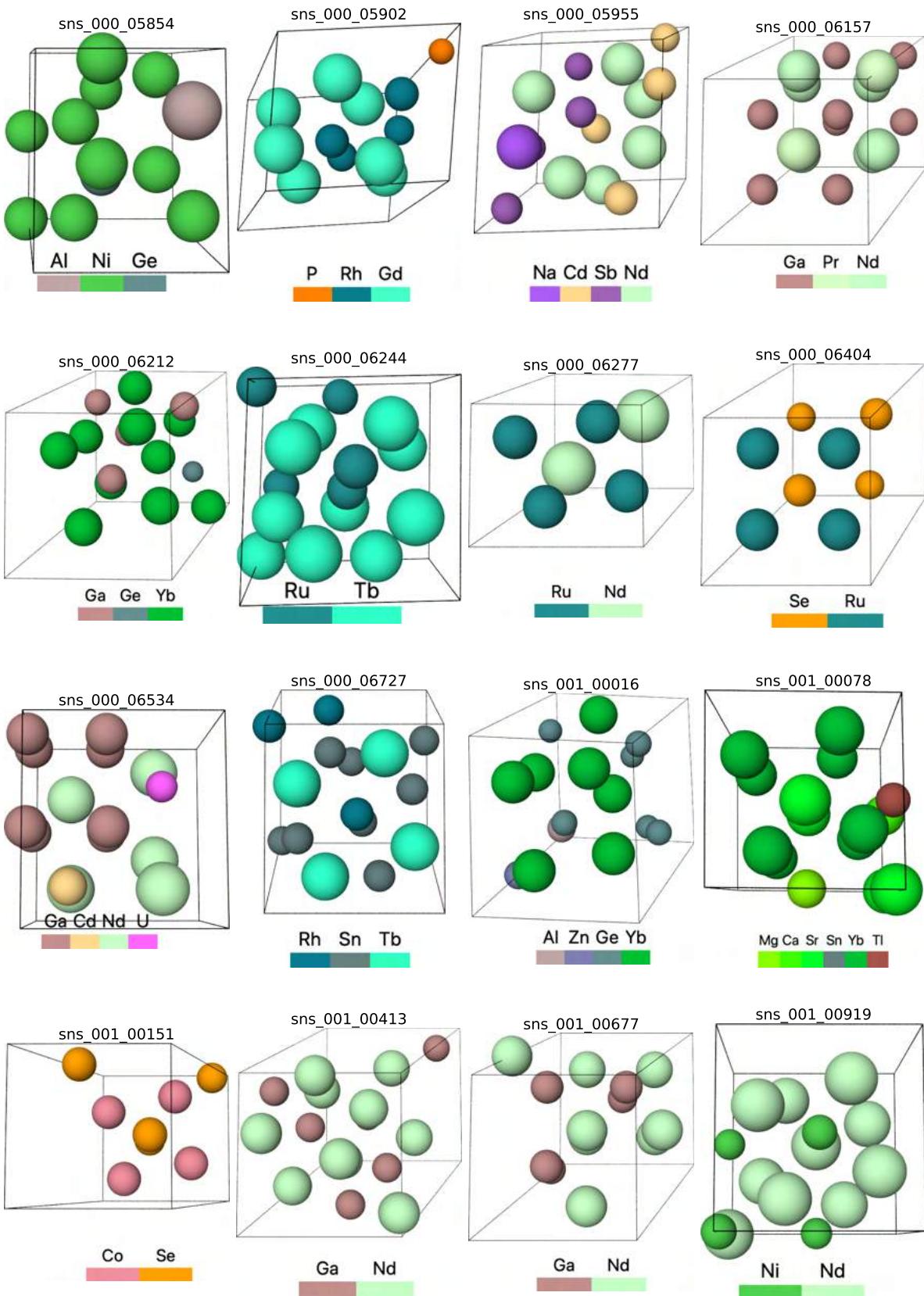


Figure S149. Generated materials with Snub square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

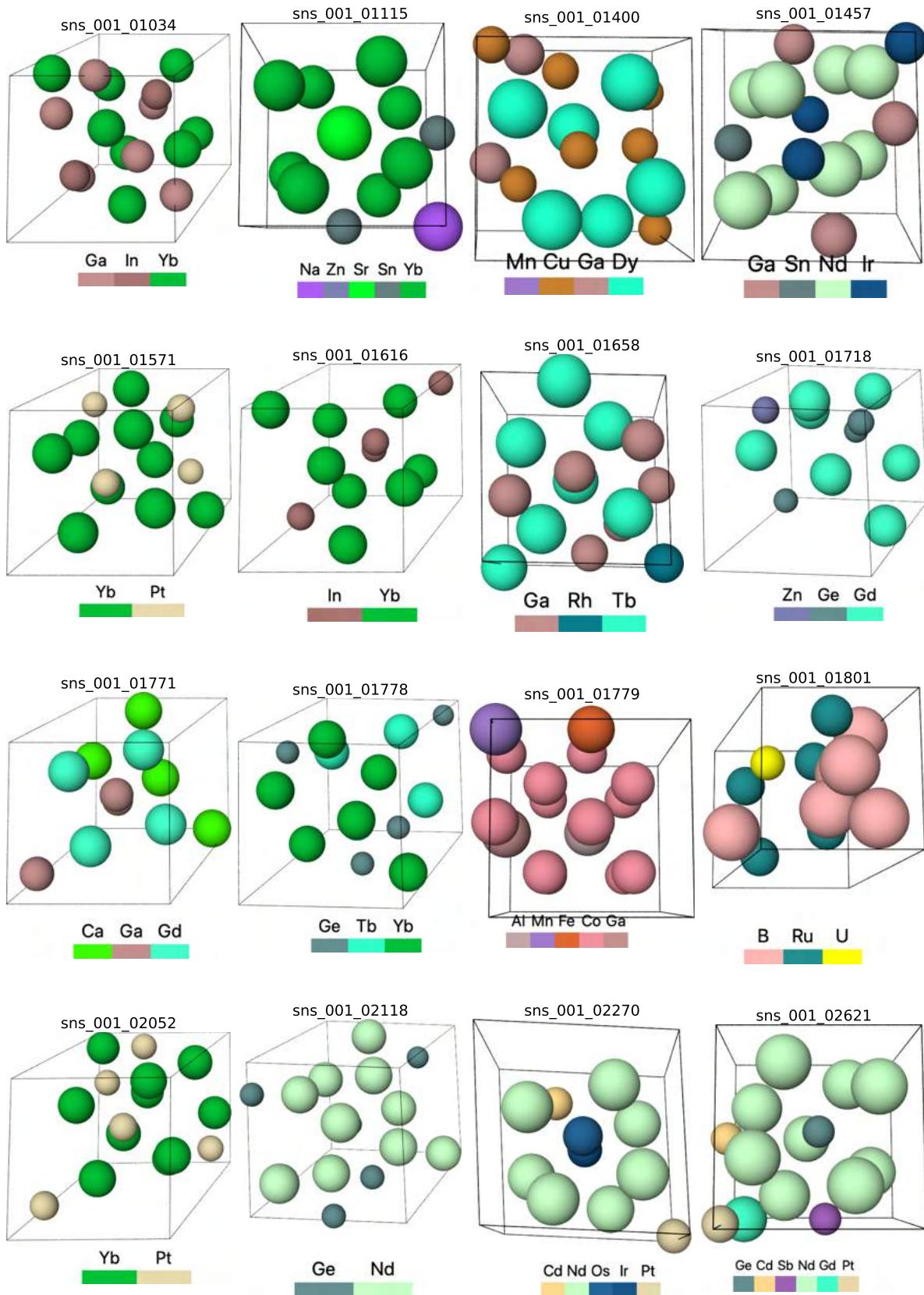


Figure S150. Generated materials with Snub square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

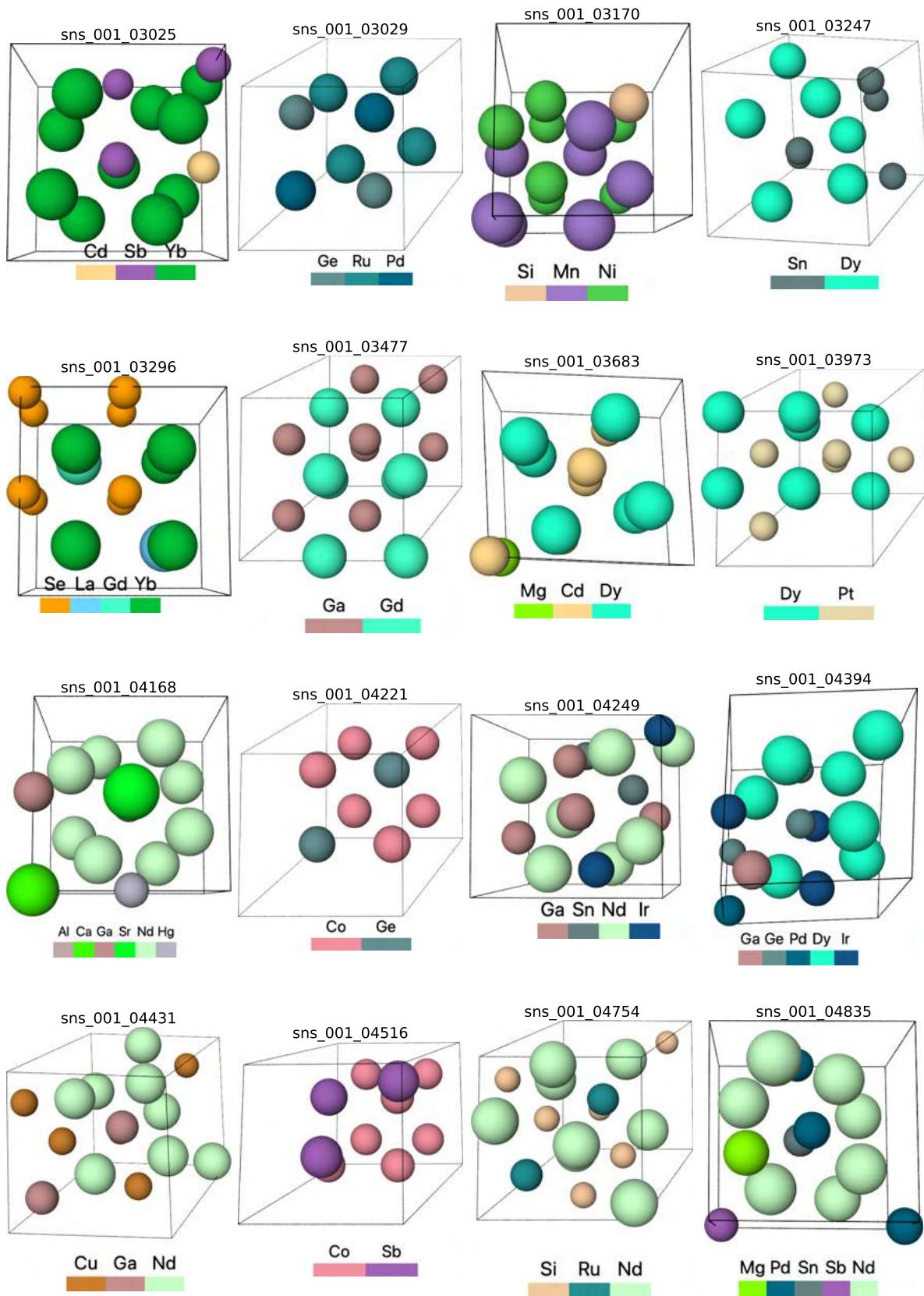


Figure S151. Generated materials with Snub square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

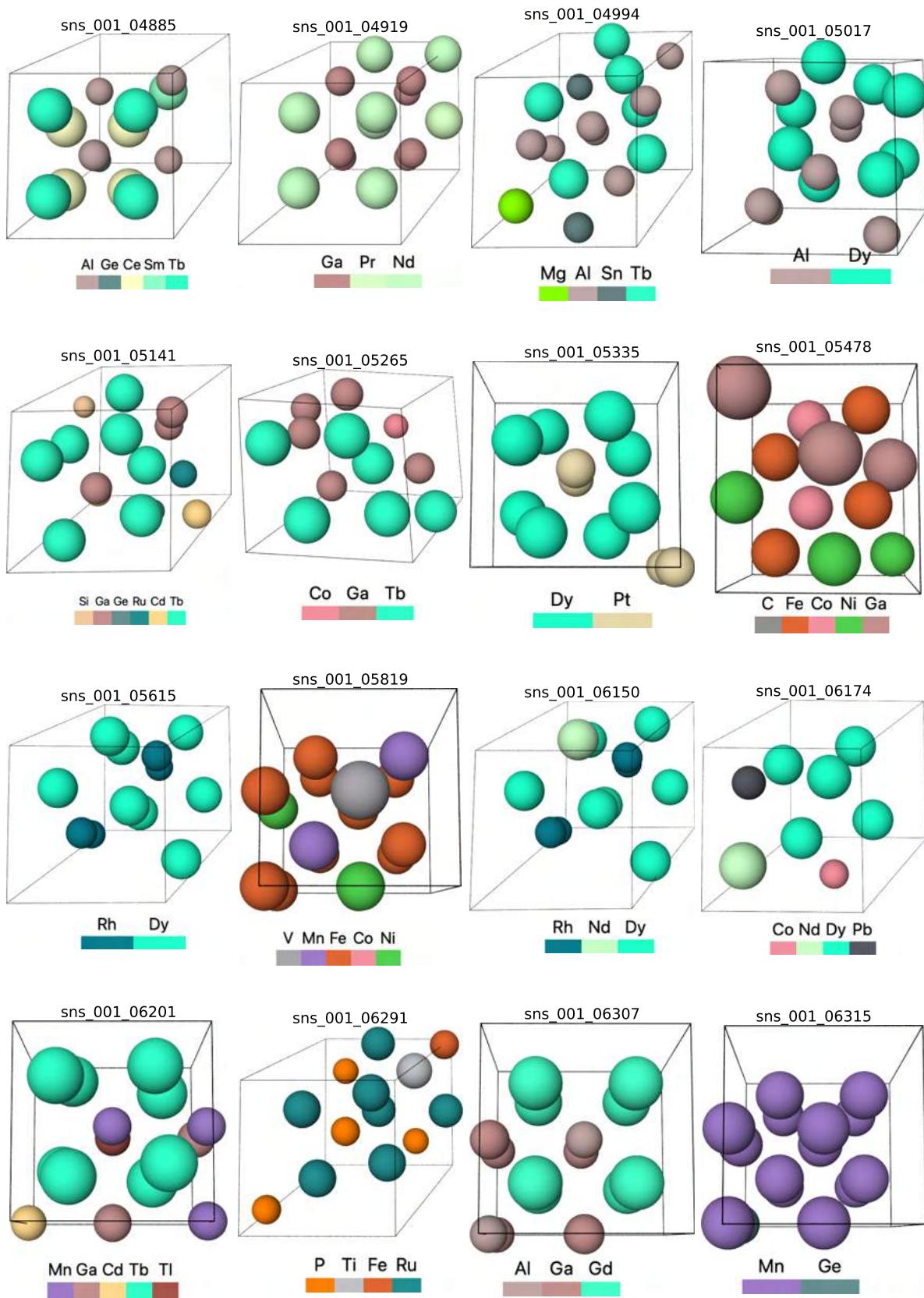


Figure S152. Generated materials with Snub square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

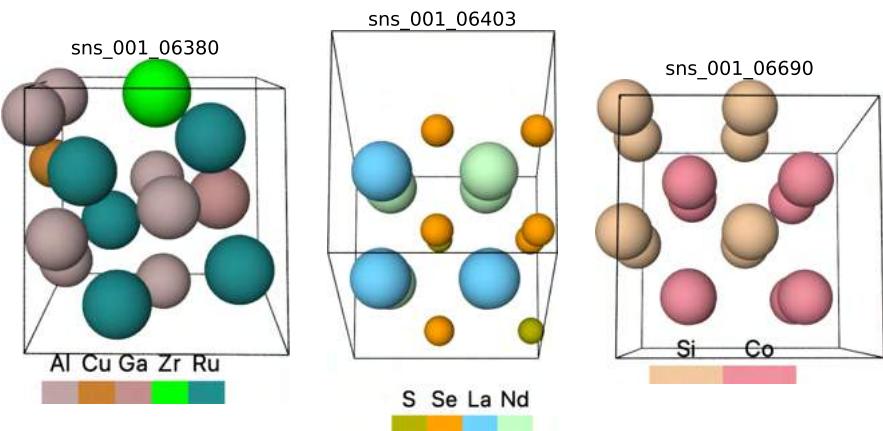


Figure S153. Generated materials with Snub square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

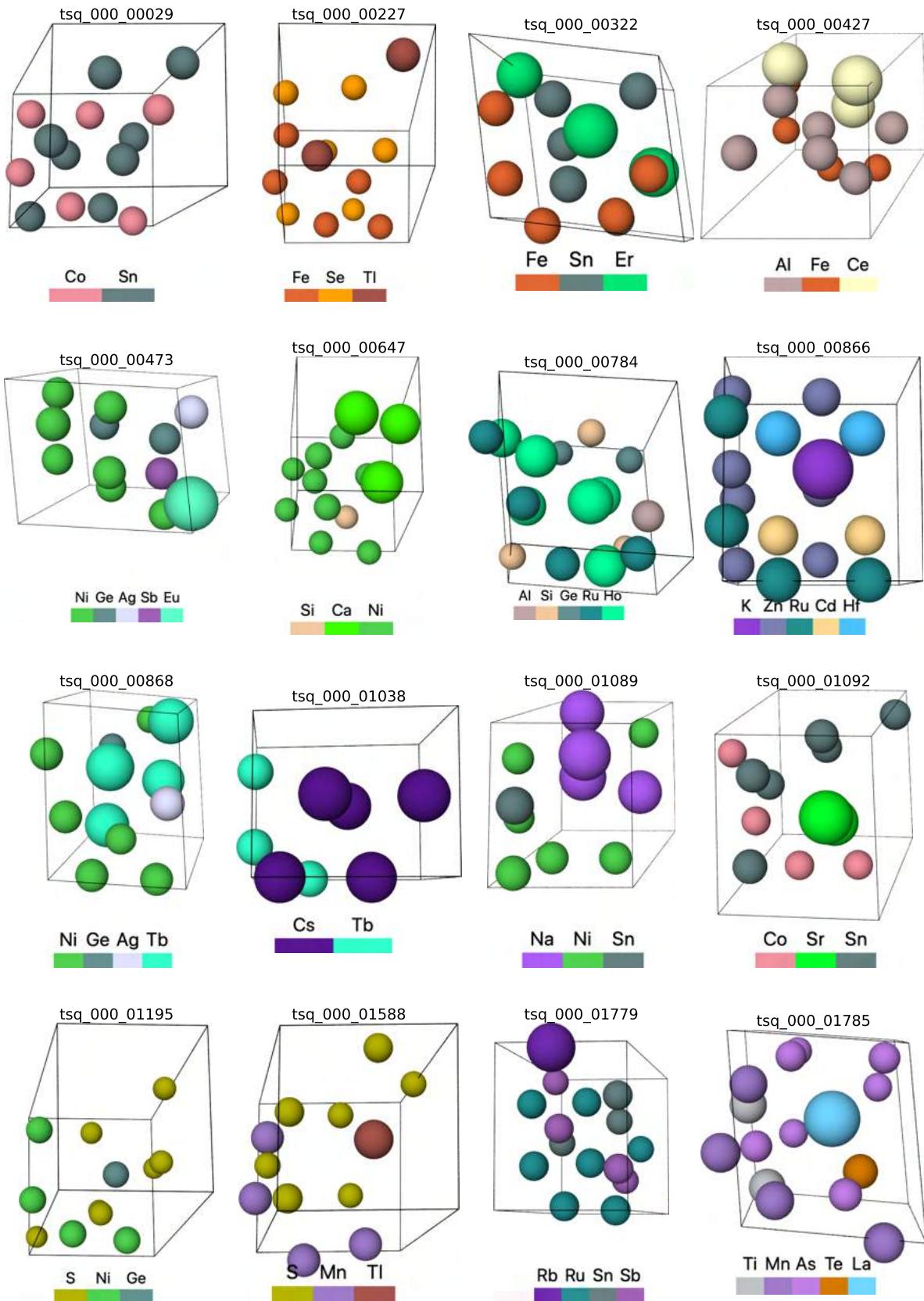


Figure S154. Generated materials with Truncated square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

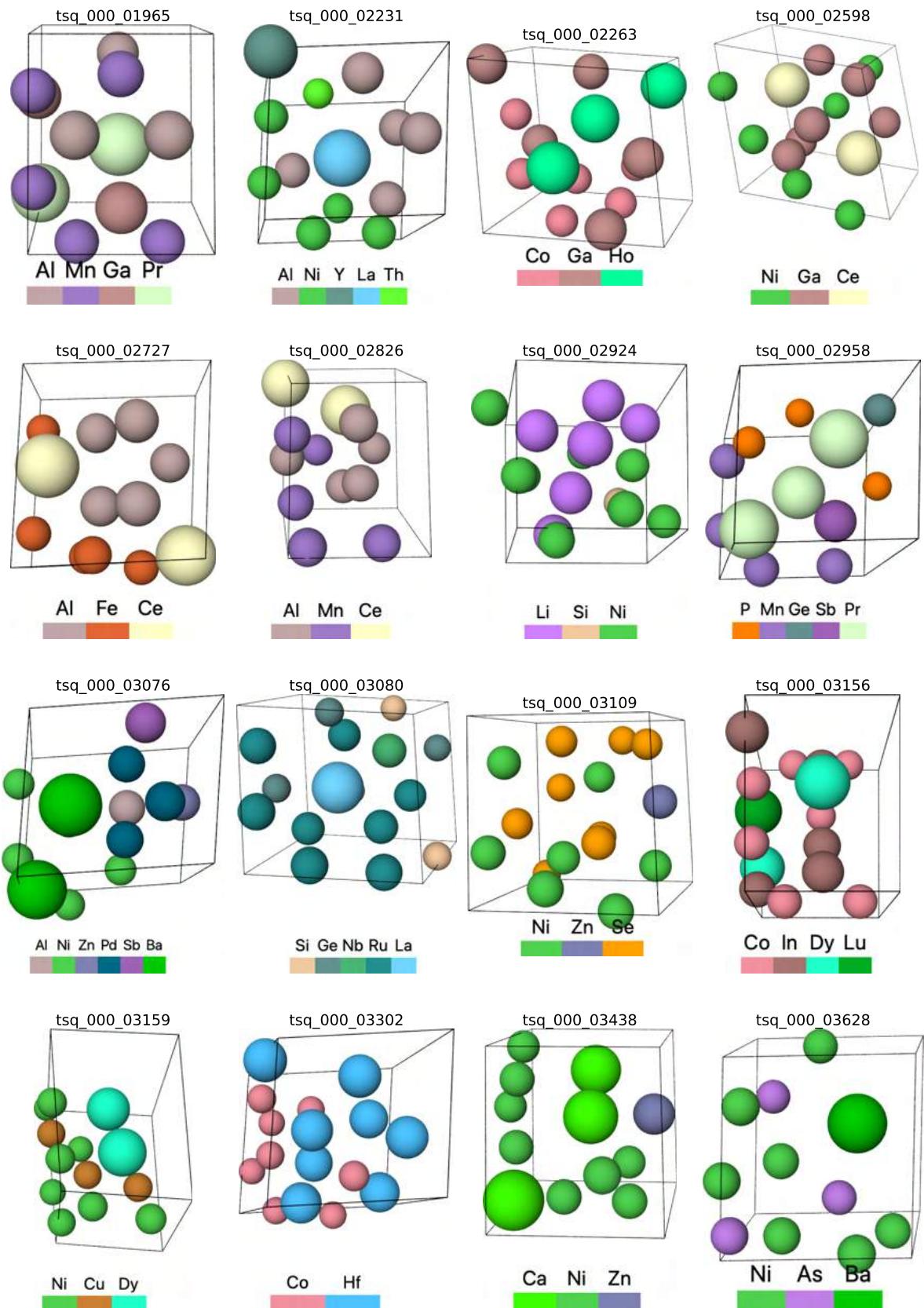


Figure S155. Generated materials with Truncated square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

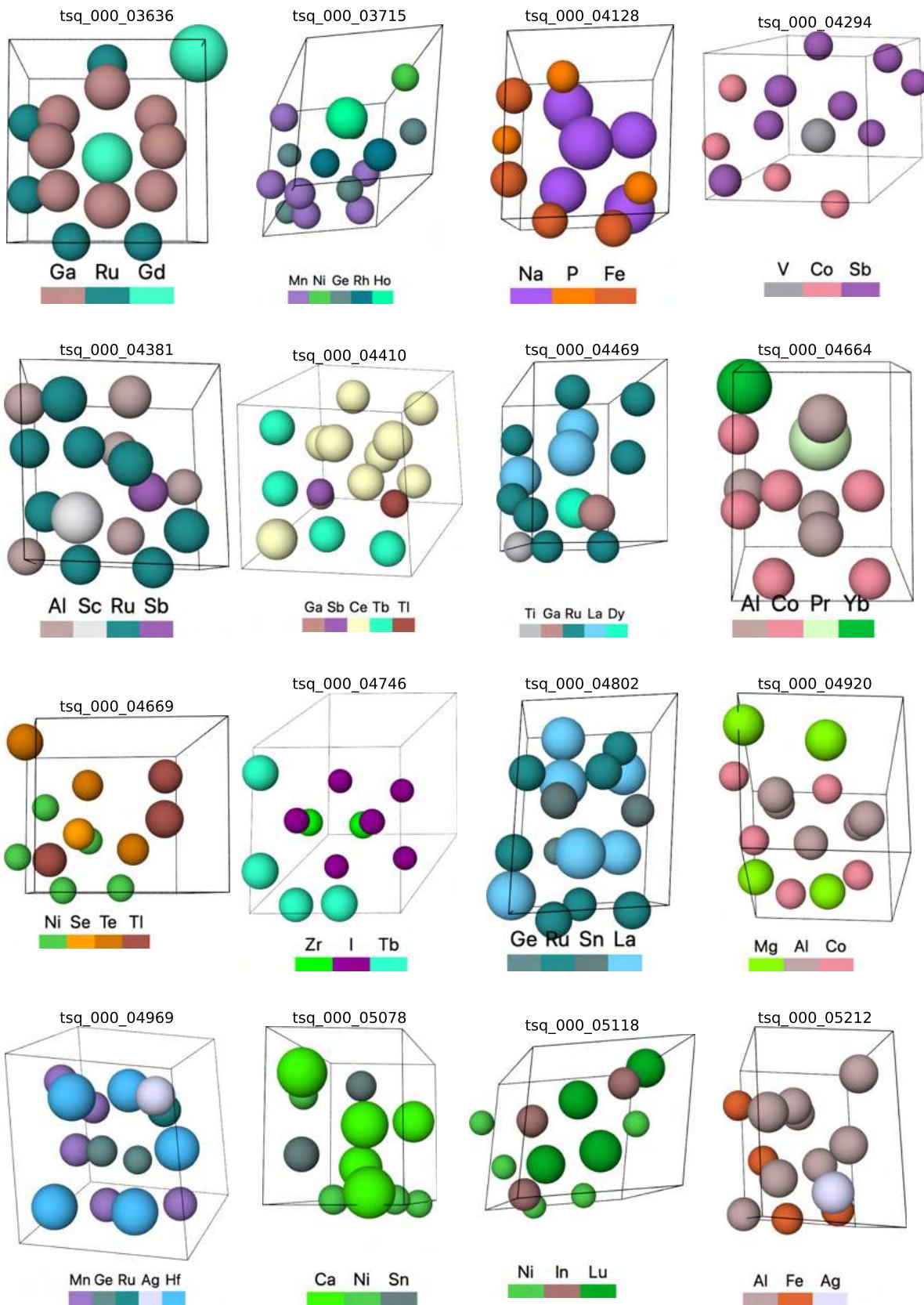


Figure S156. Generated materials with Truncated square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

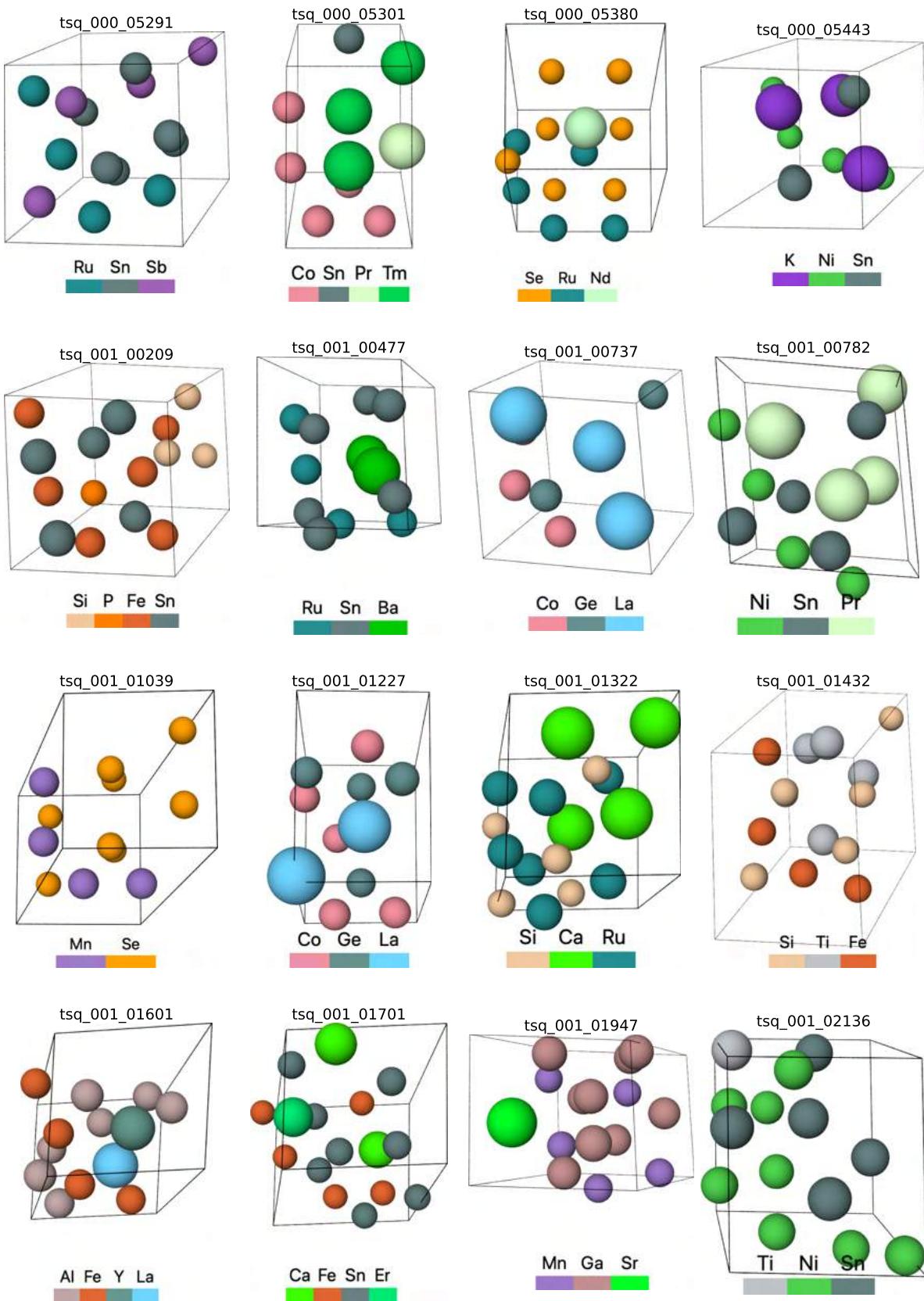


Figure S157. Generated materials with Truncated square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

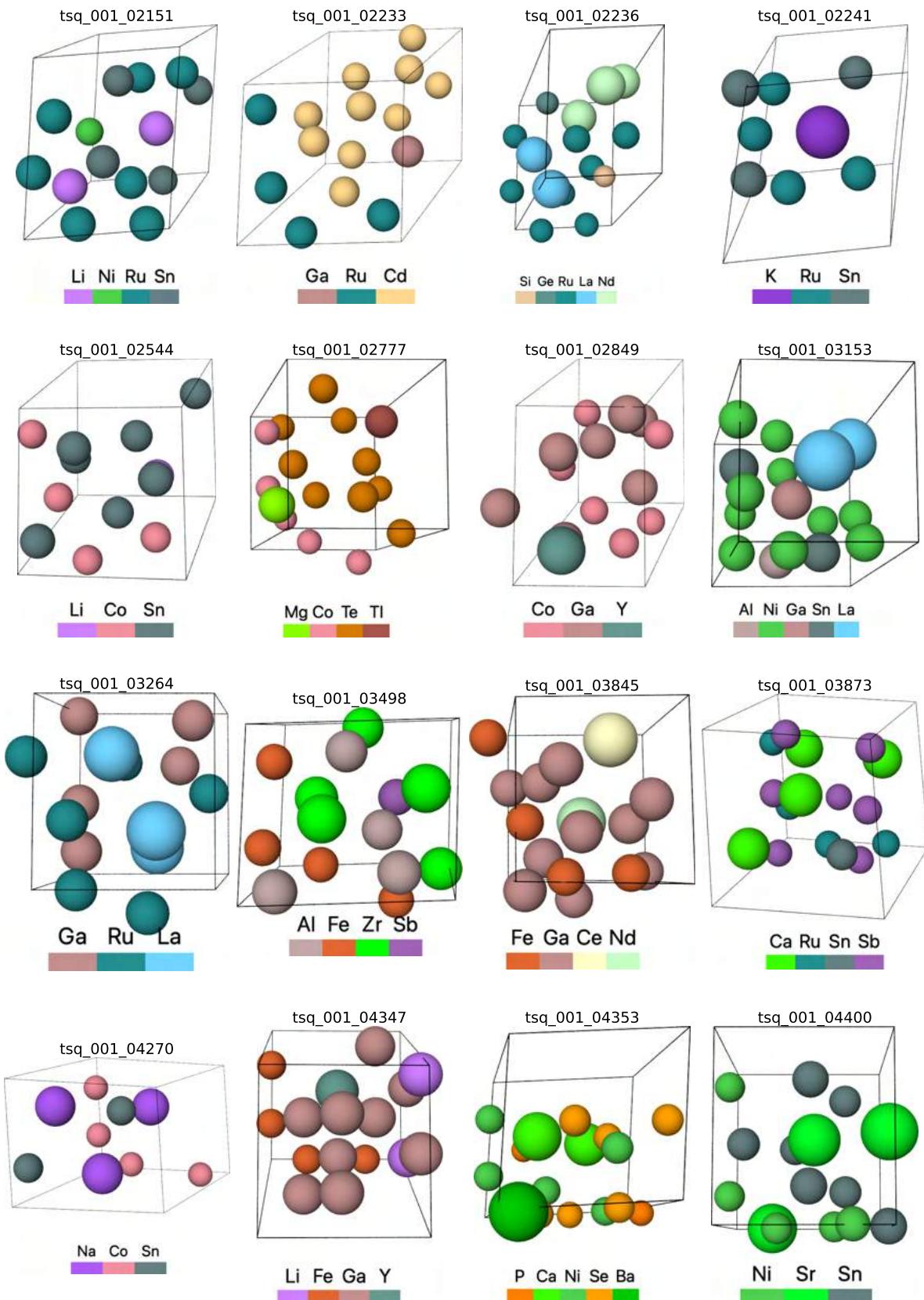


Figure S158. Generated materials with Truncated square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

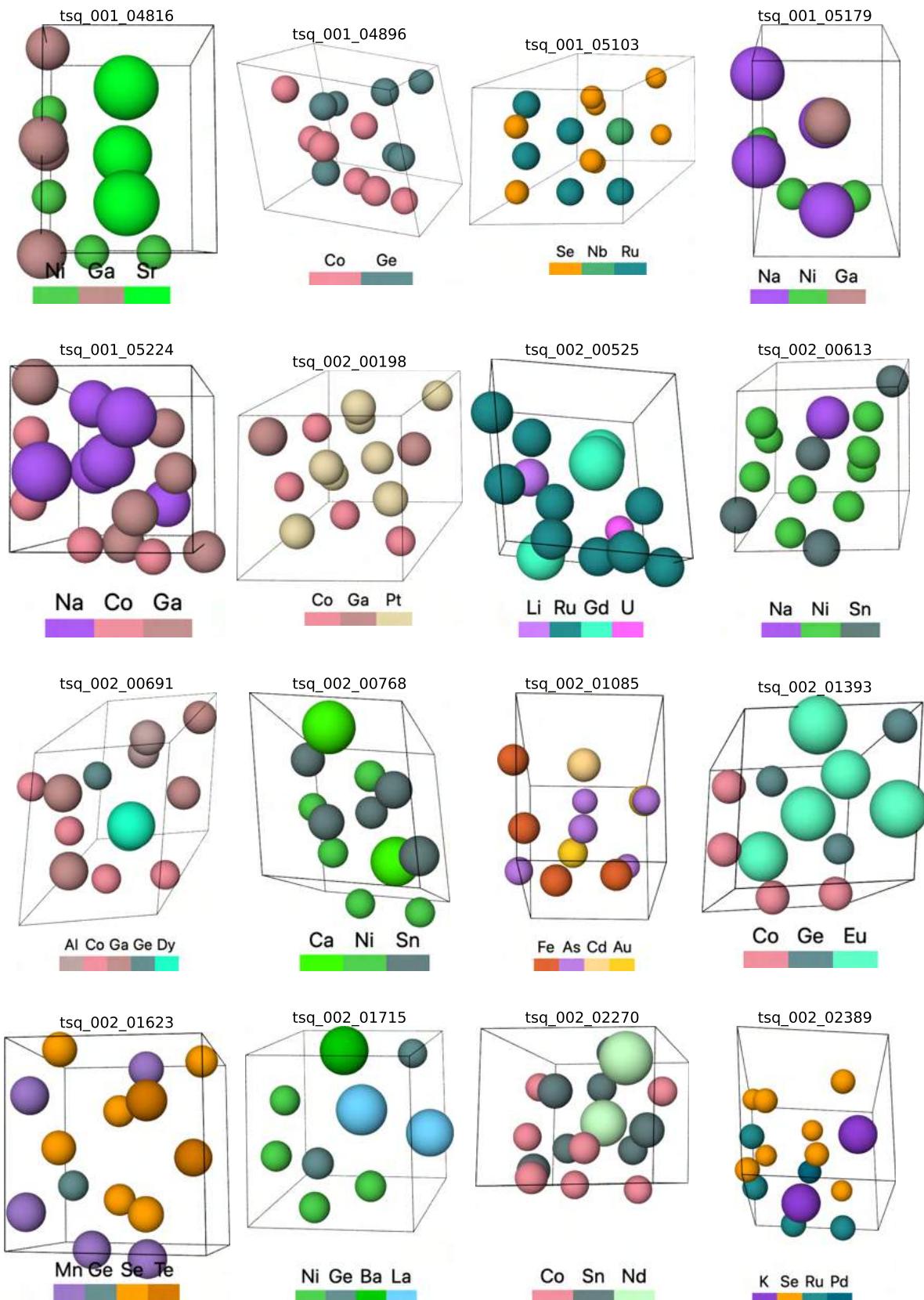


Figure S159. Generated materials with Truncated square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

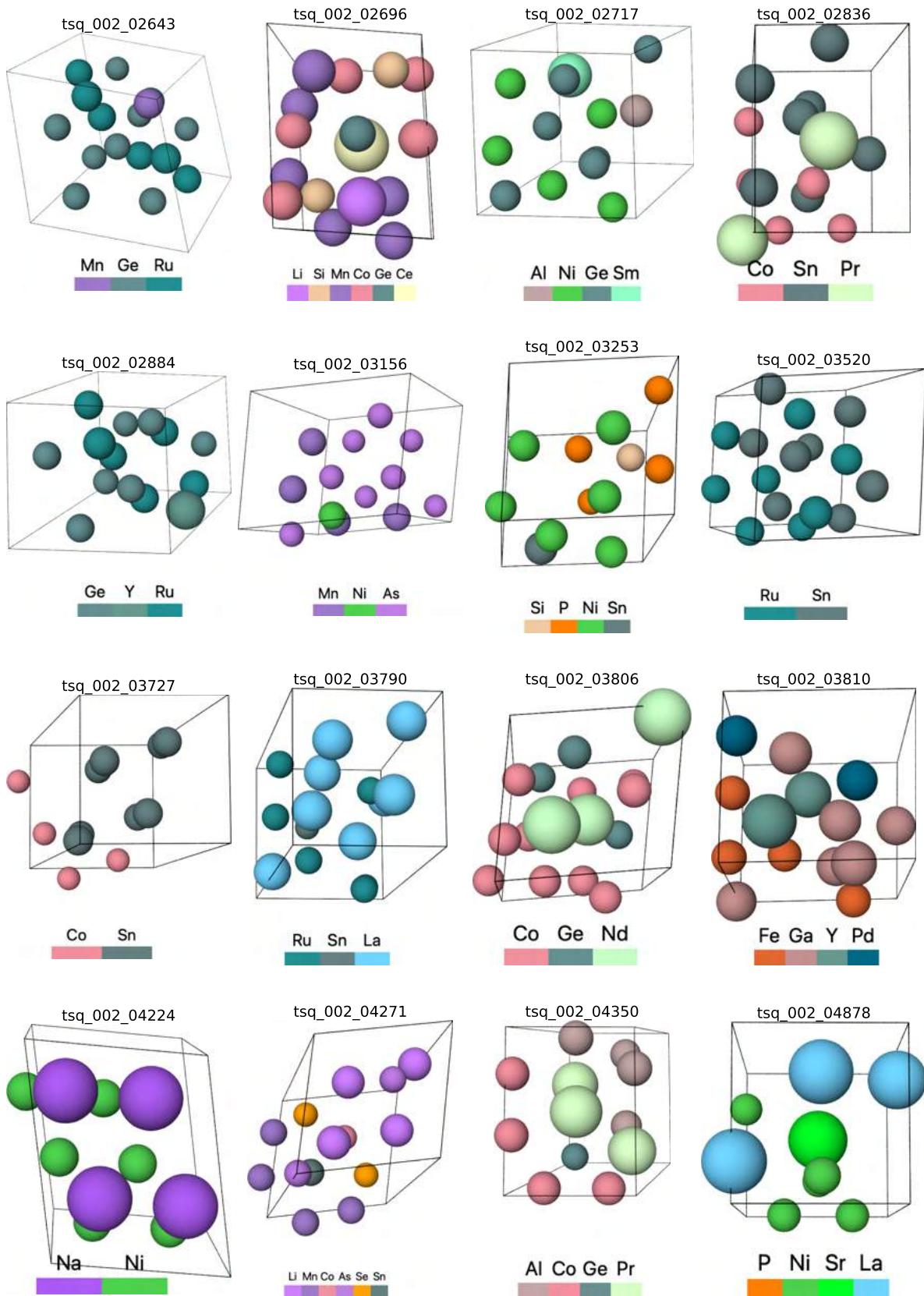


Figure S160. Generated materials with Truncated square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

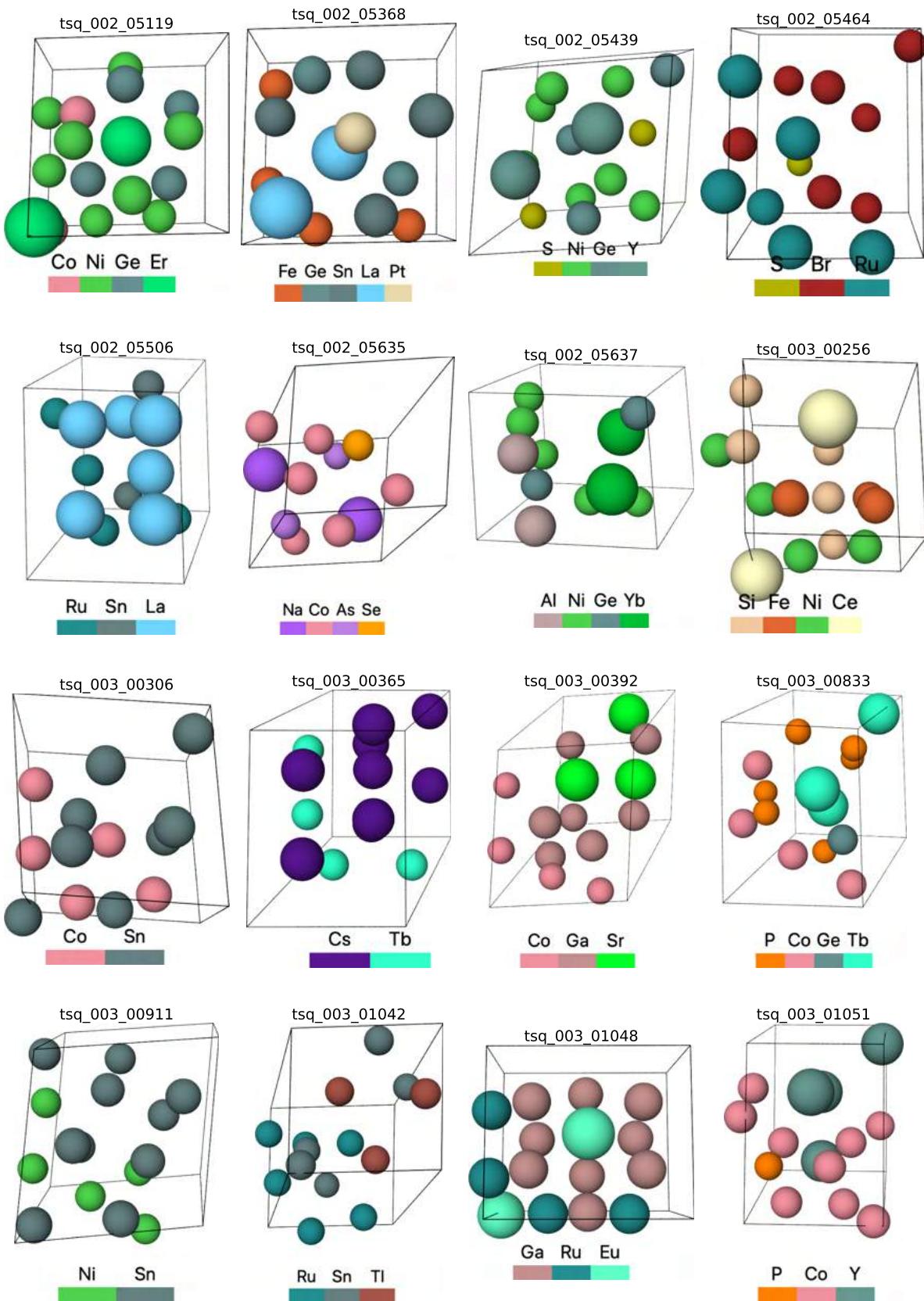


Figure S161. Generated materials with Truncated square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

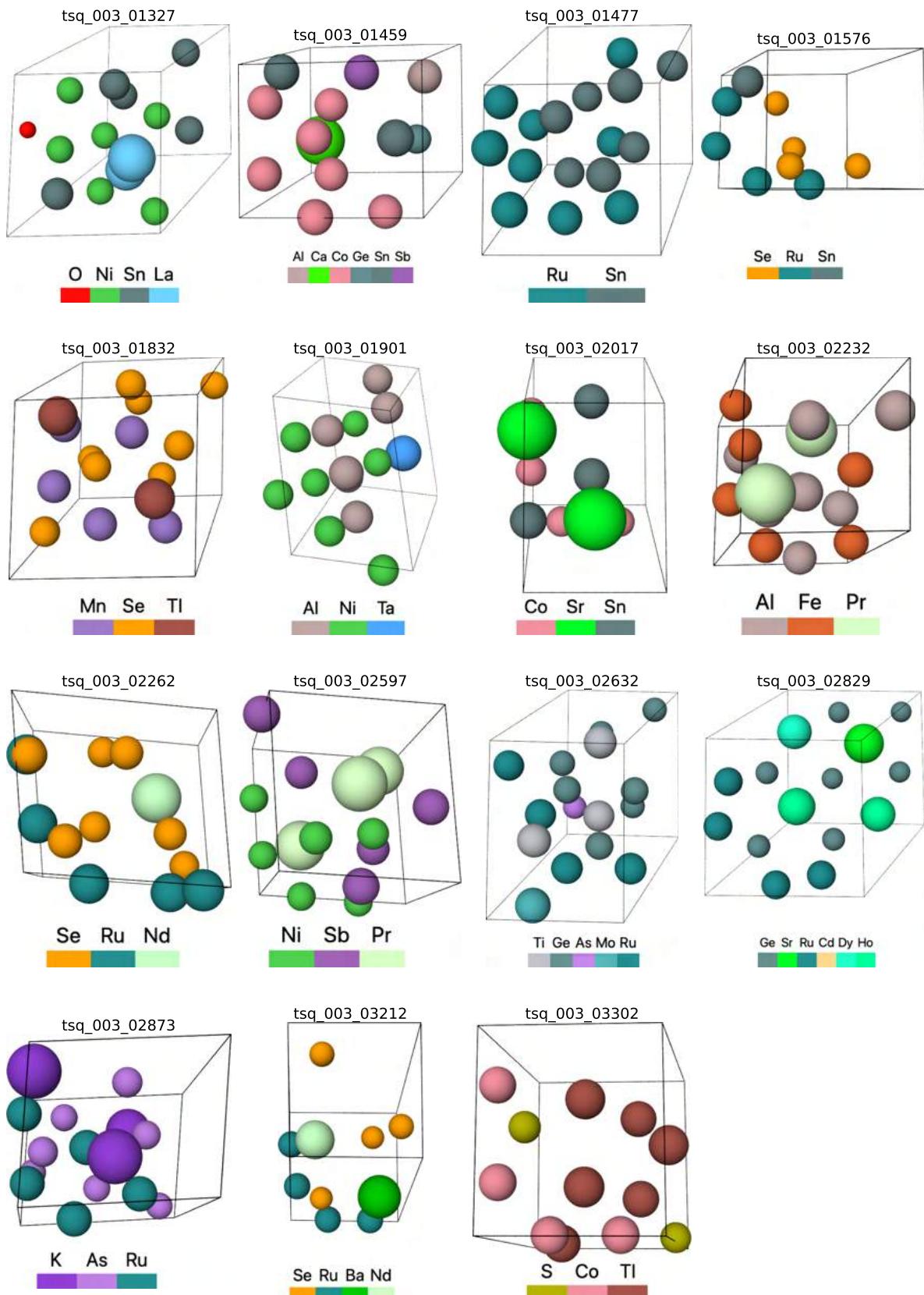


Figure S162. Generated materials with Truncated square lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

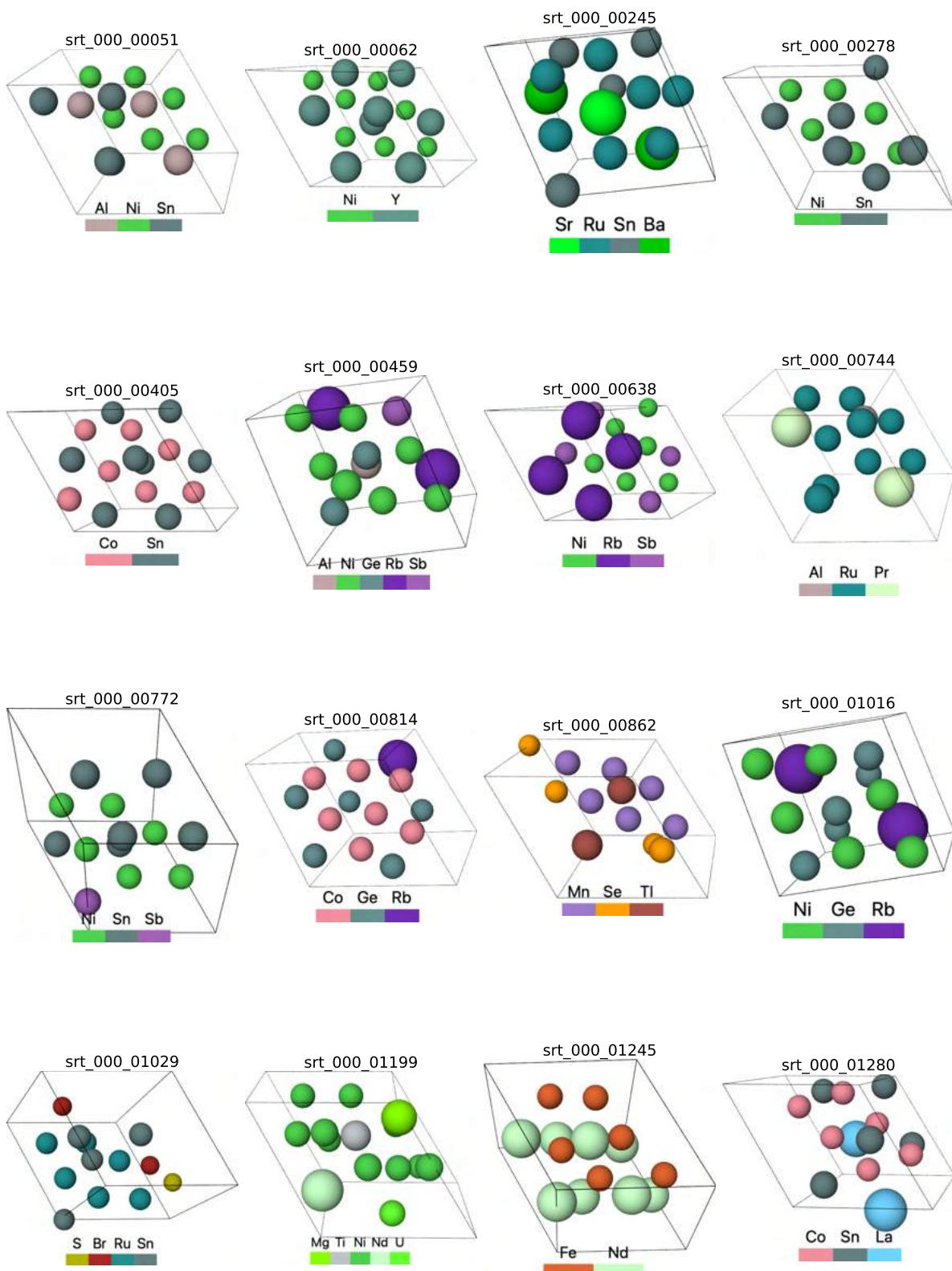


Figure S163. Generated materials with Small rhombitrihexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

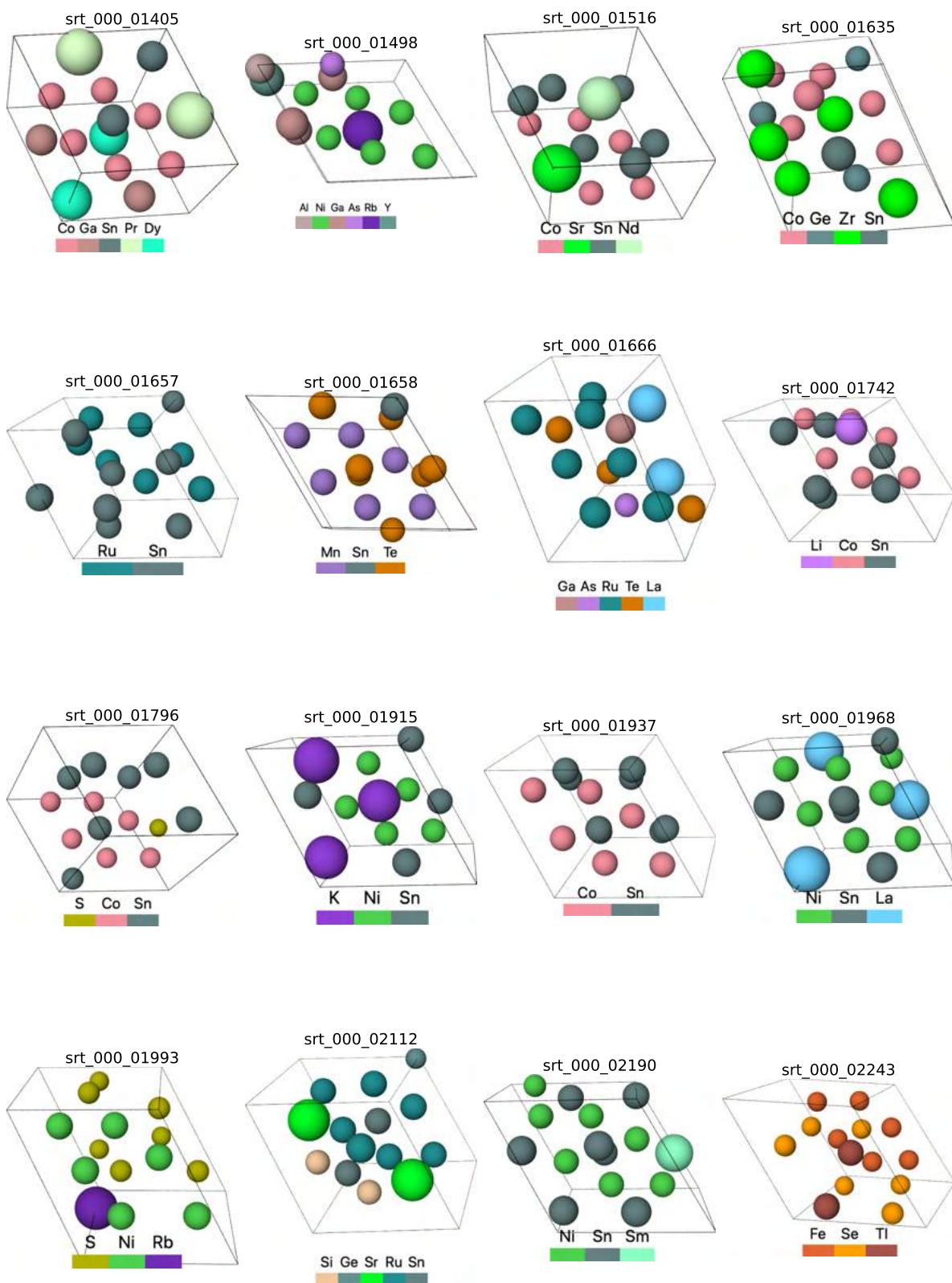


Figure S164. Generated materials with Small rhombitrihexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

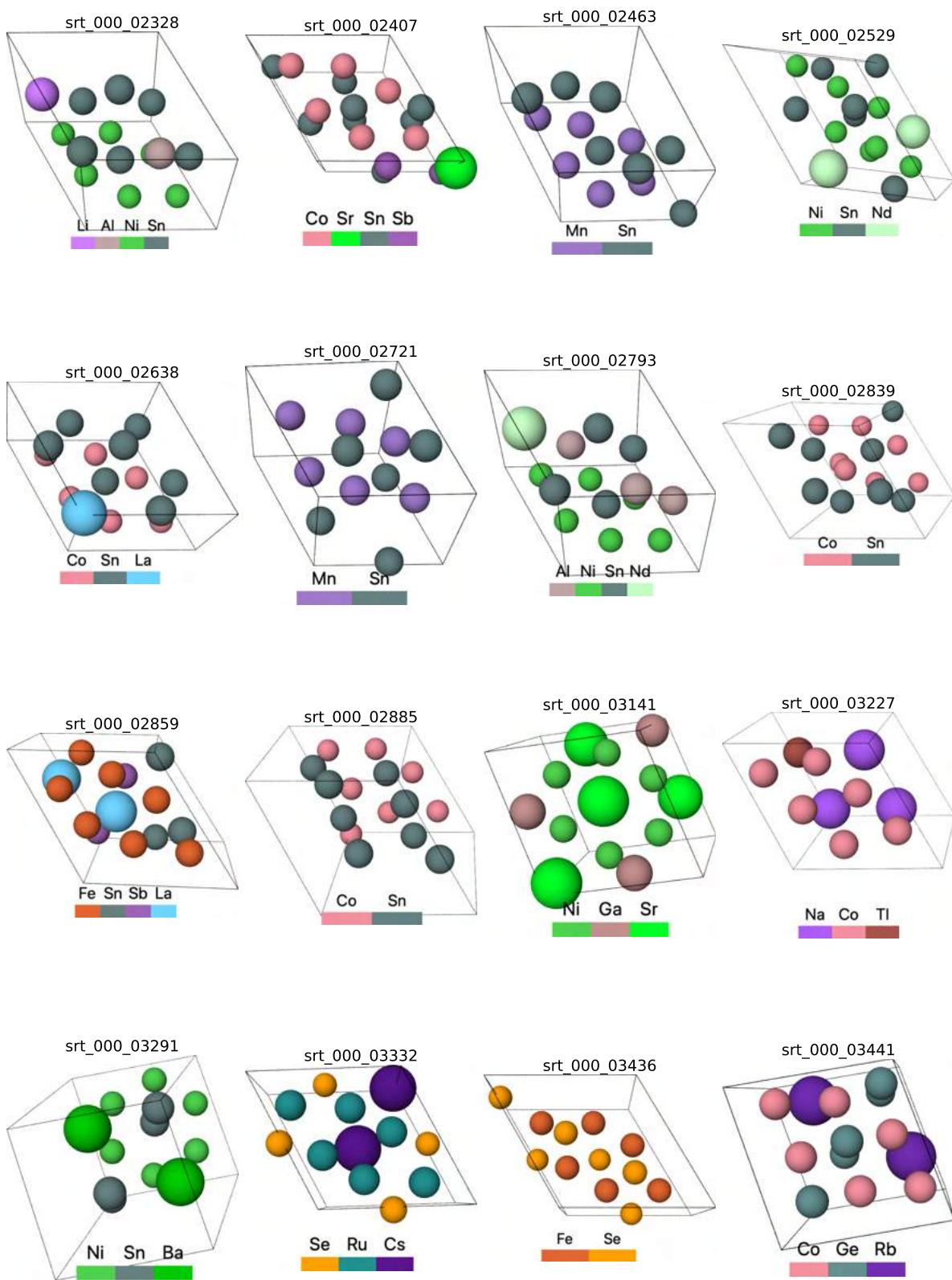


Figure S165. Generated materials with Small rhombitrihexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

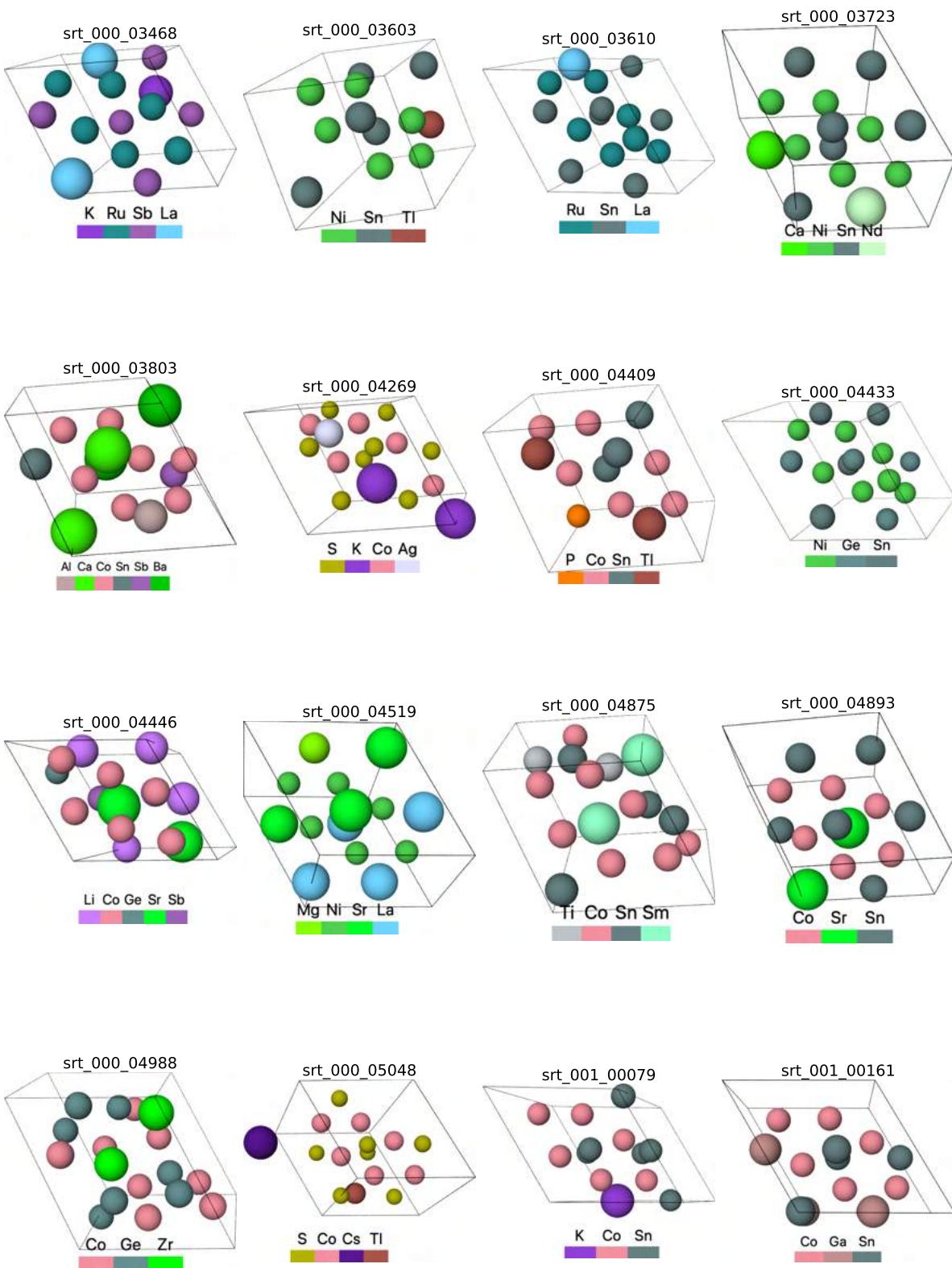


Figure S166. Generated materials with Small rhombitrihexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

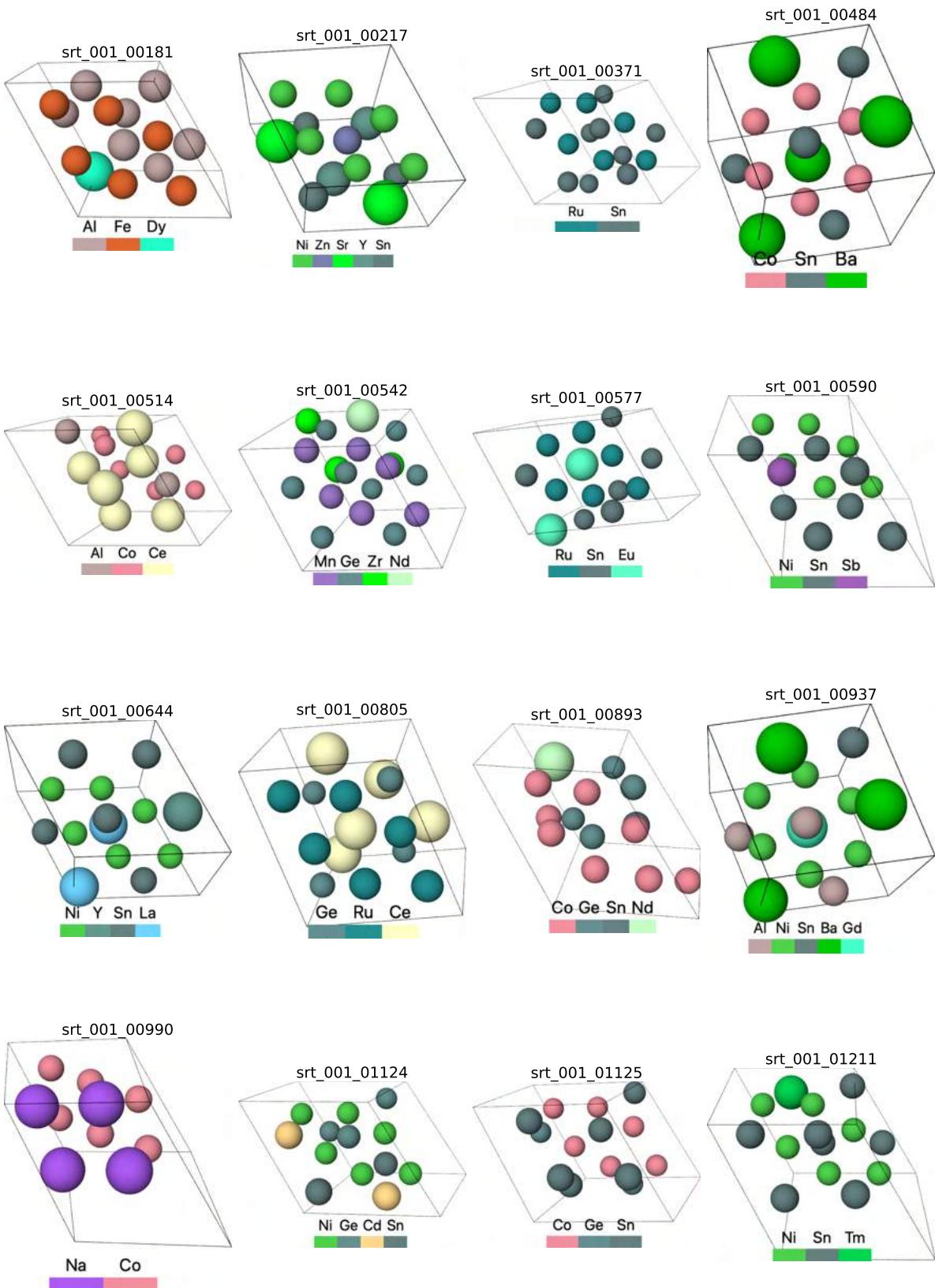


Figure S167. Generated materials with Small rhombitrihexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

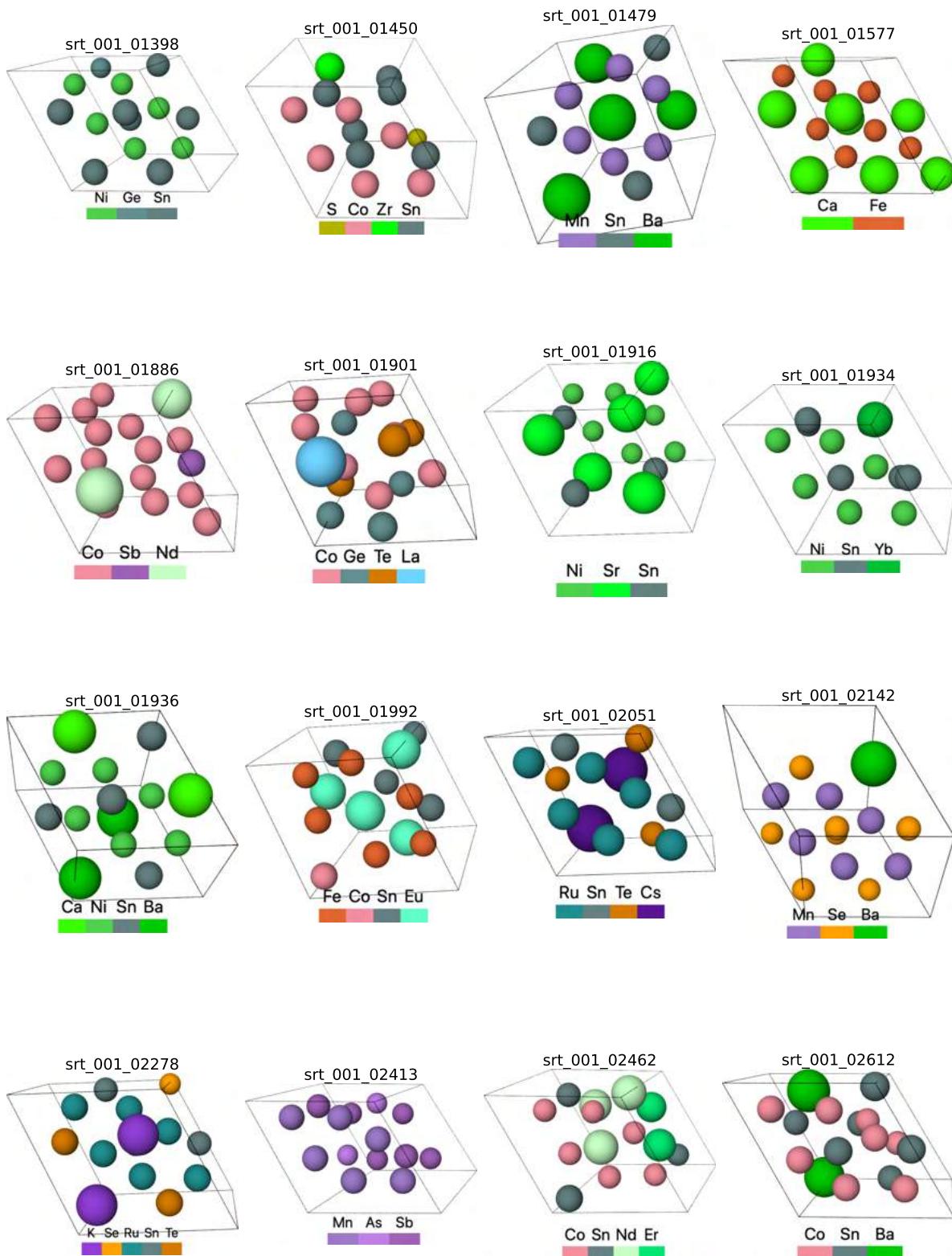


Figure S168. Generated materials with Small rhombitrihexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

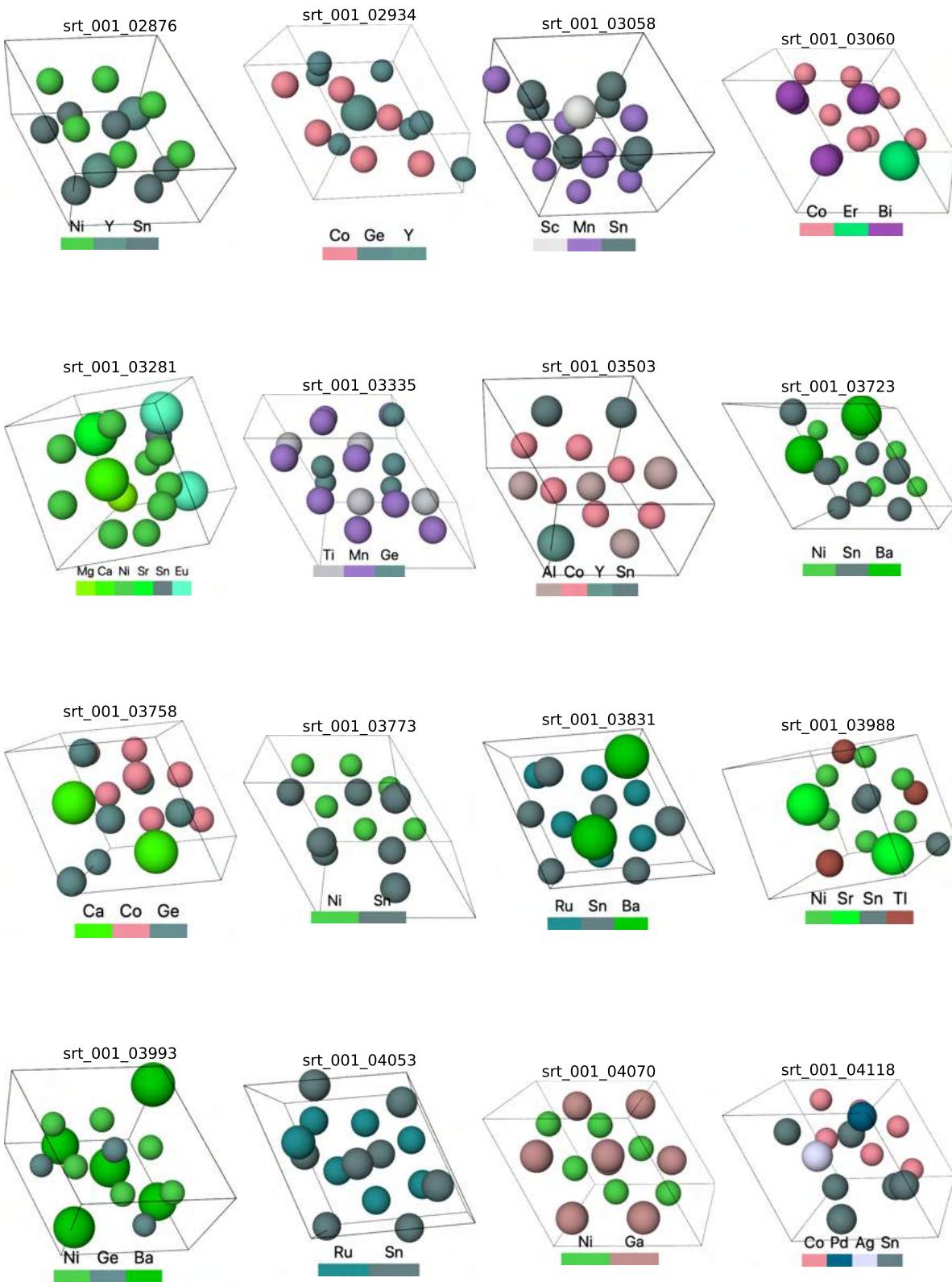


Figure S169. Generated materials with Small rhombitrihexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

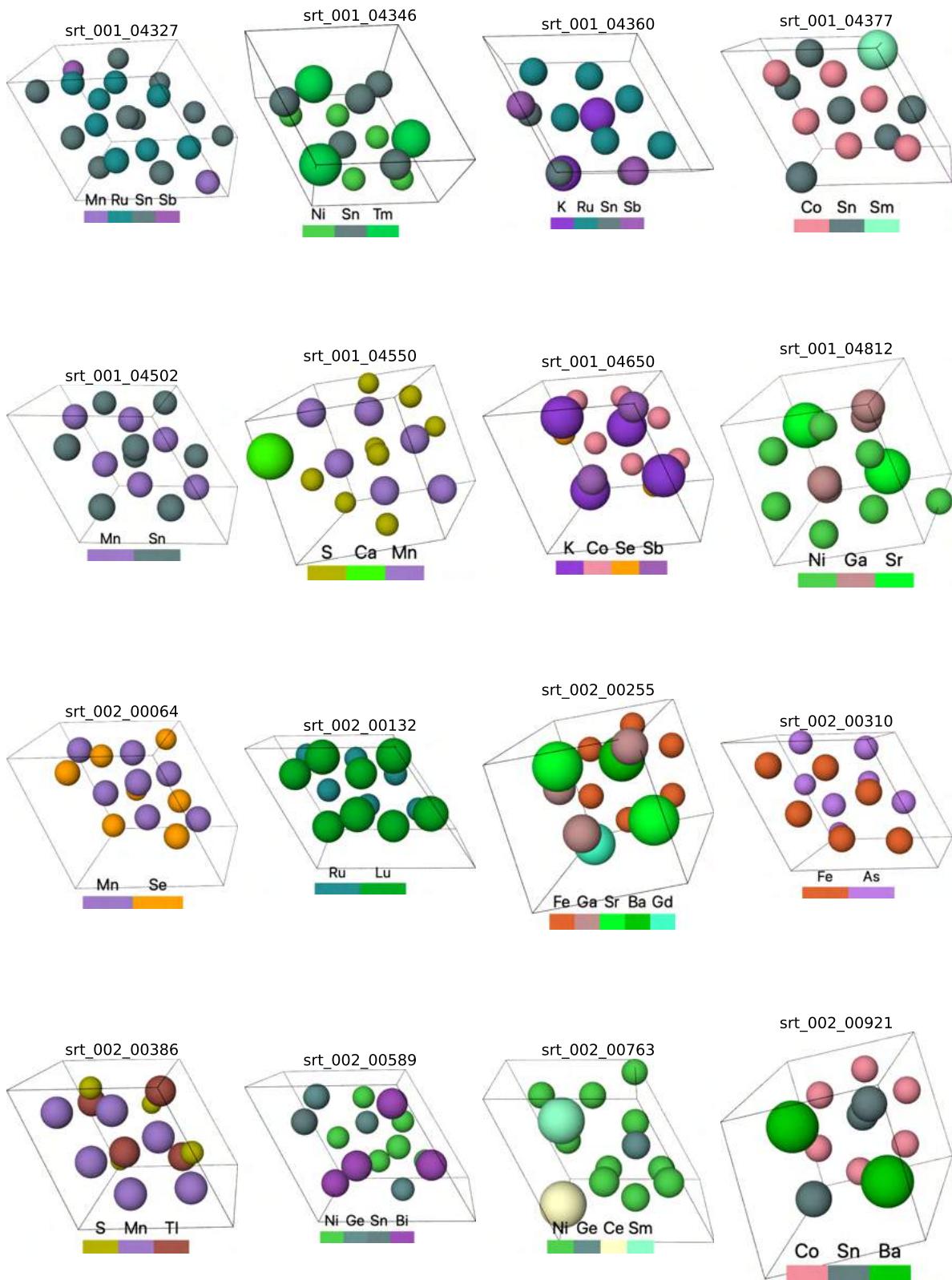


Figure S170. Generated materials with Small rhombitrihexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

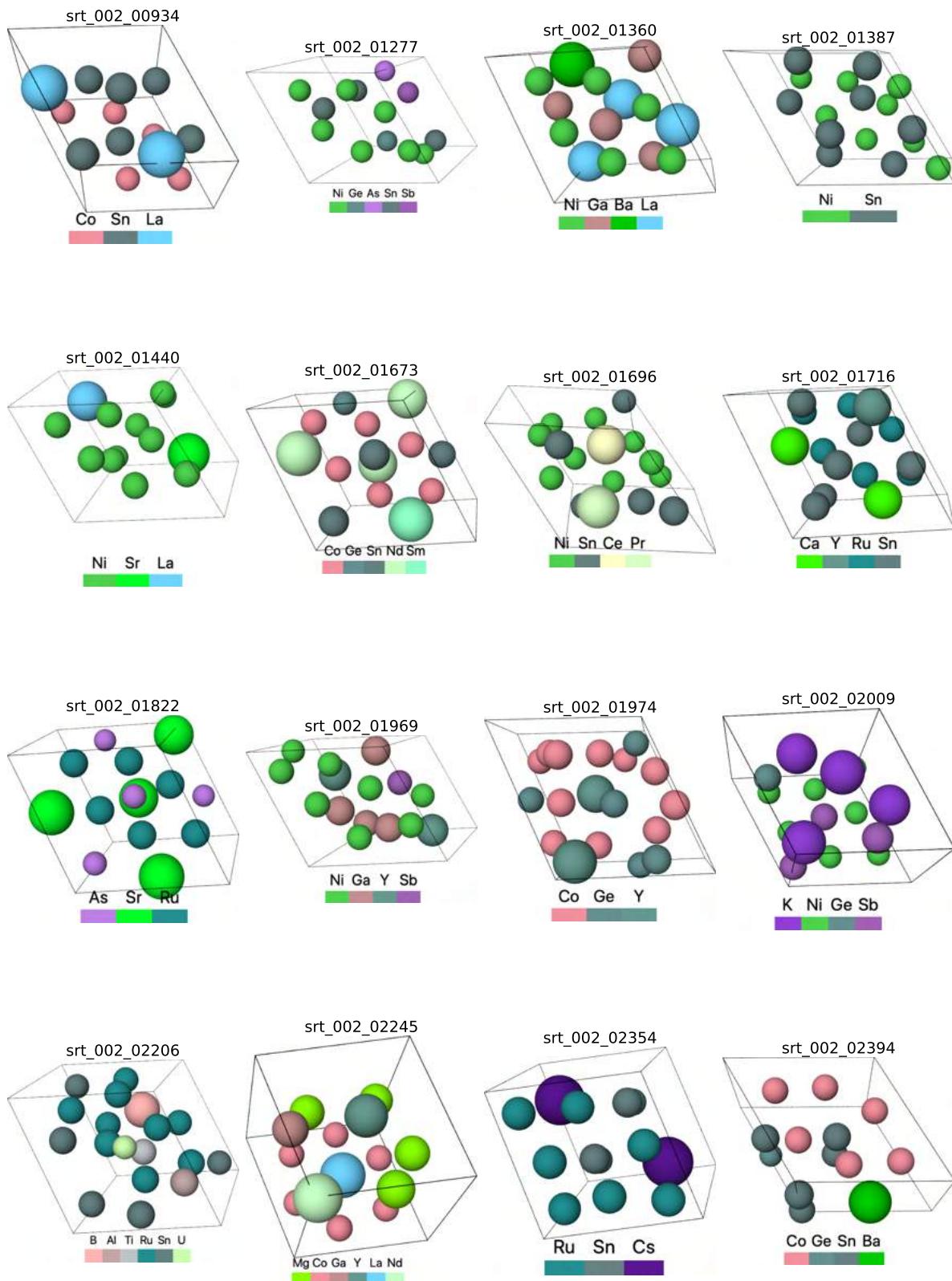


Figure S171. Generated materials with Small rhombitrihexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

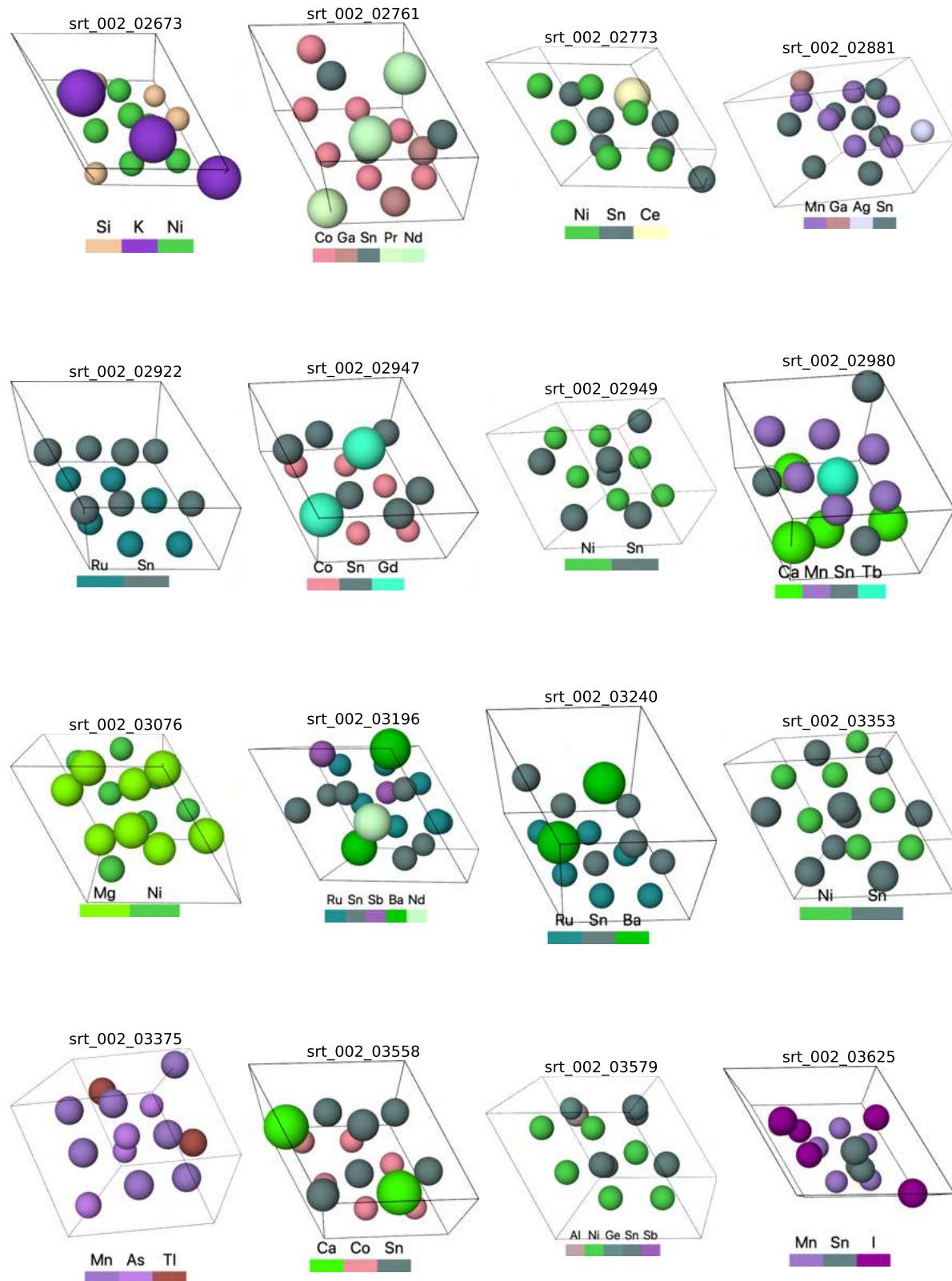


Figure S172. Generated materials with Small rhombitrihexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

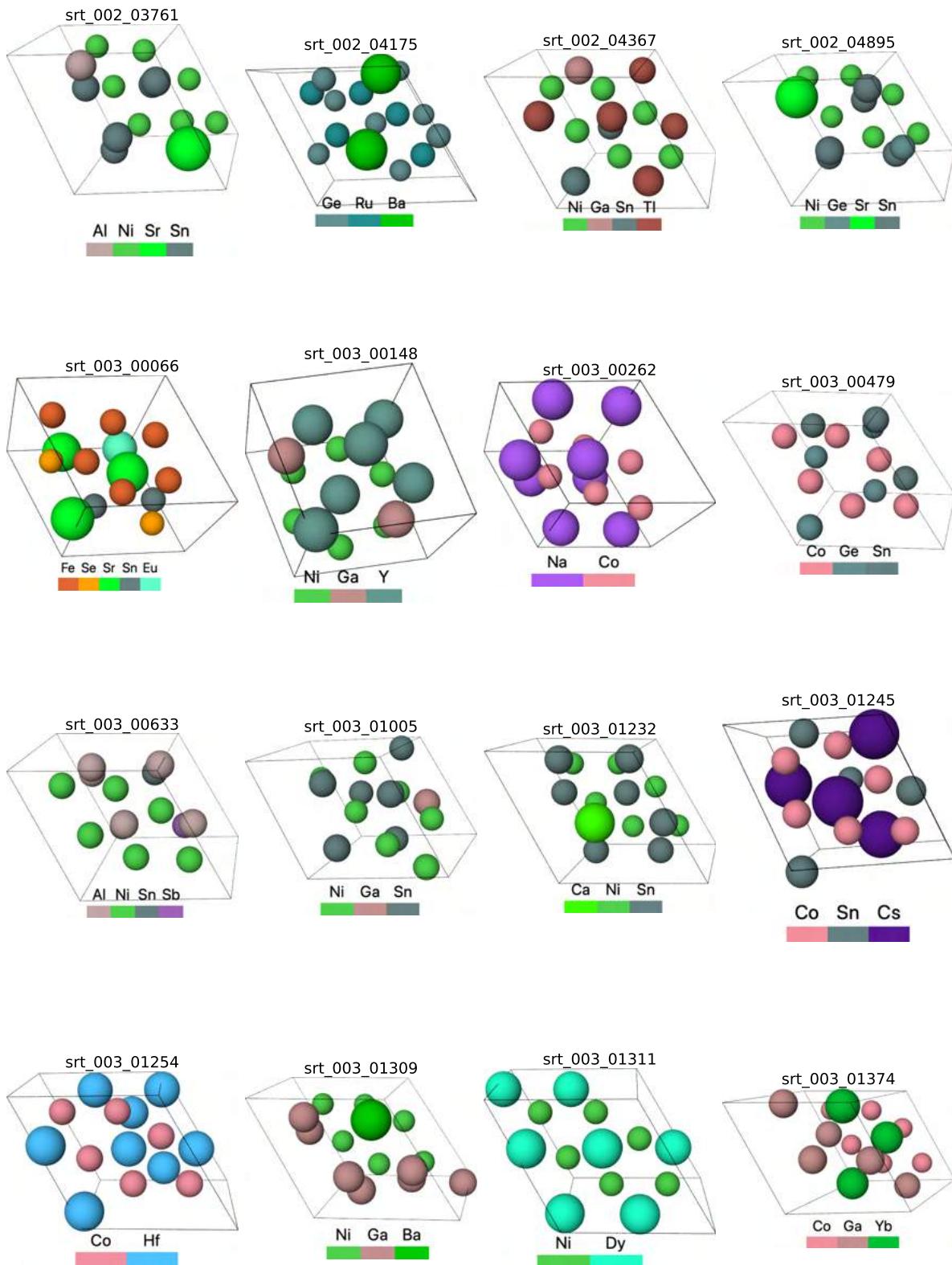


Figure S173. Generated materials with Small rhombitrihexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

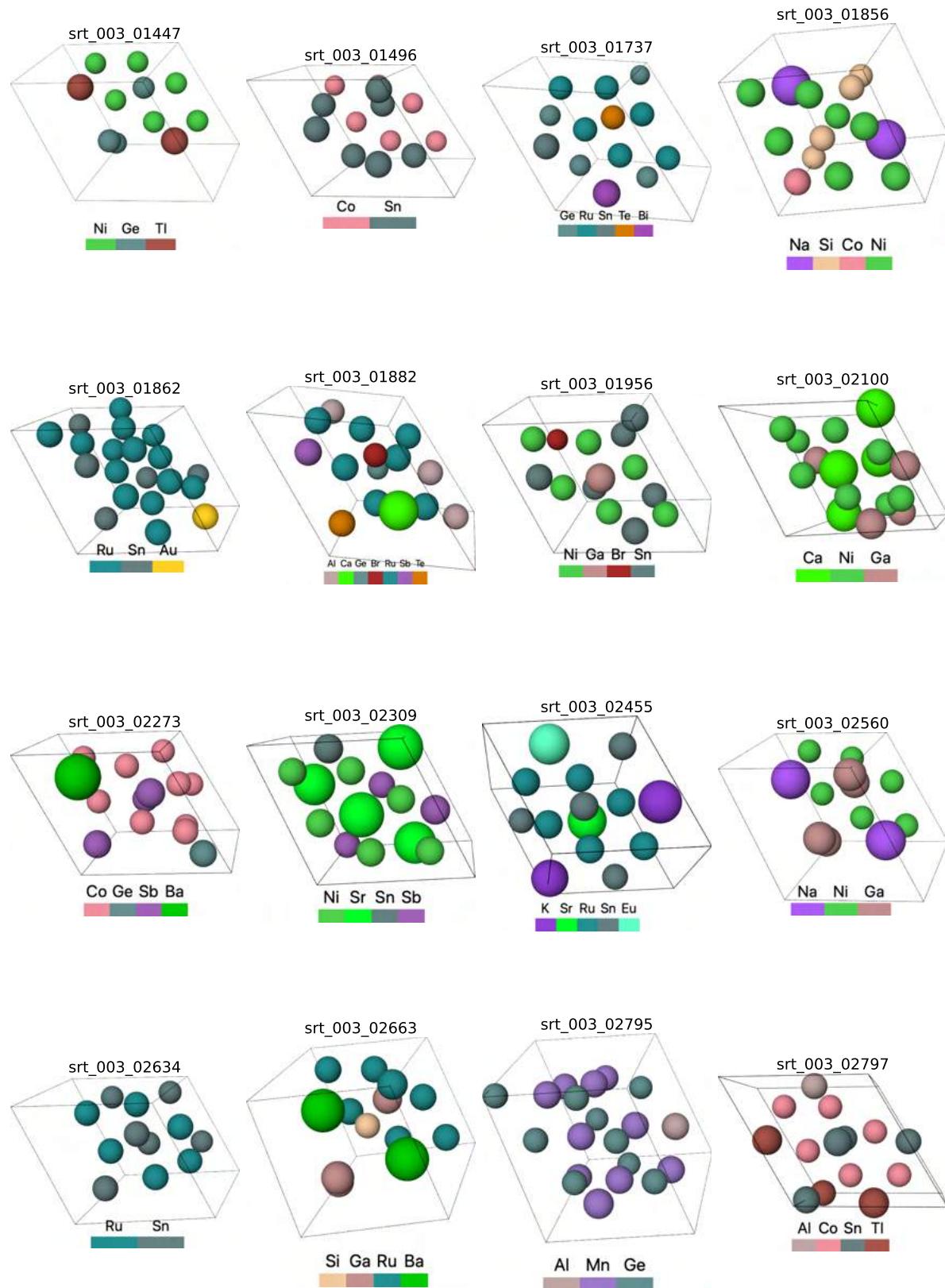


Figure S174. Generated materials with Small rhombitrihexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

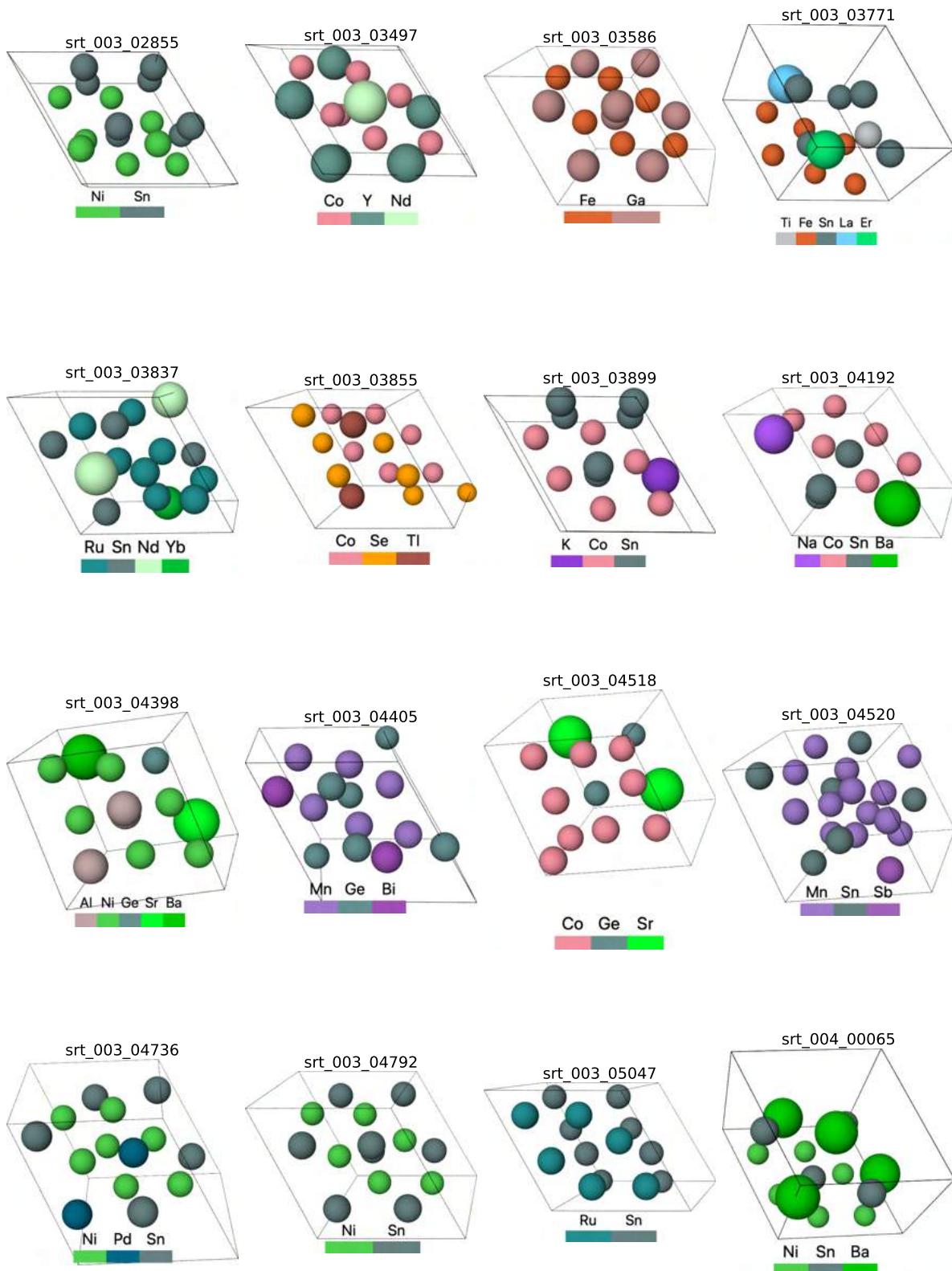


Figure S175. Generated materials with Small rhombitrihexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

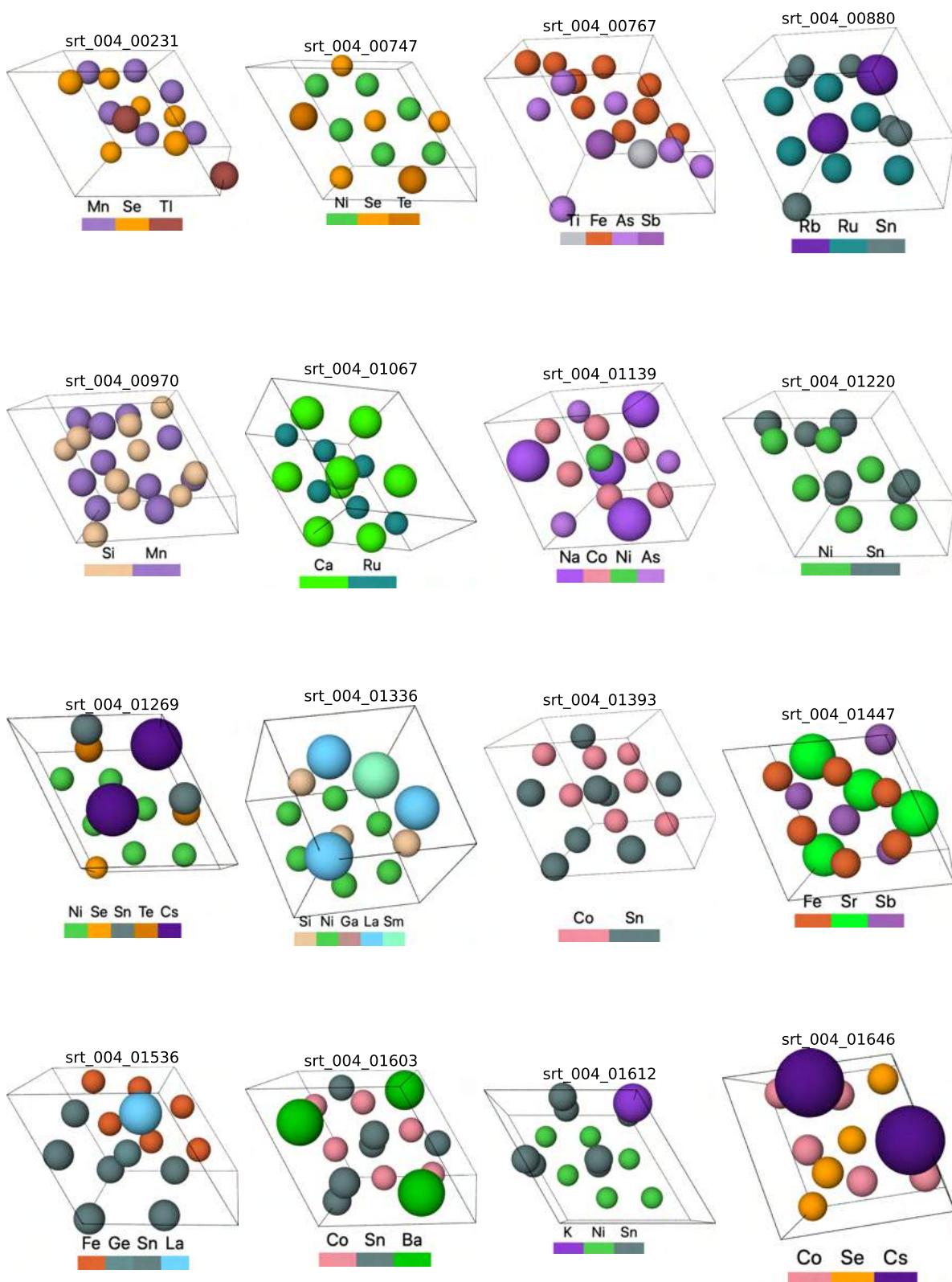


Figure S176. Generated materials with Small rhombitrihexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

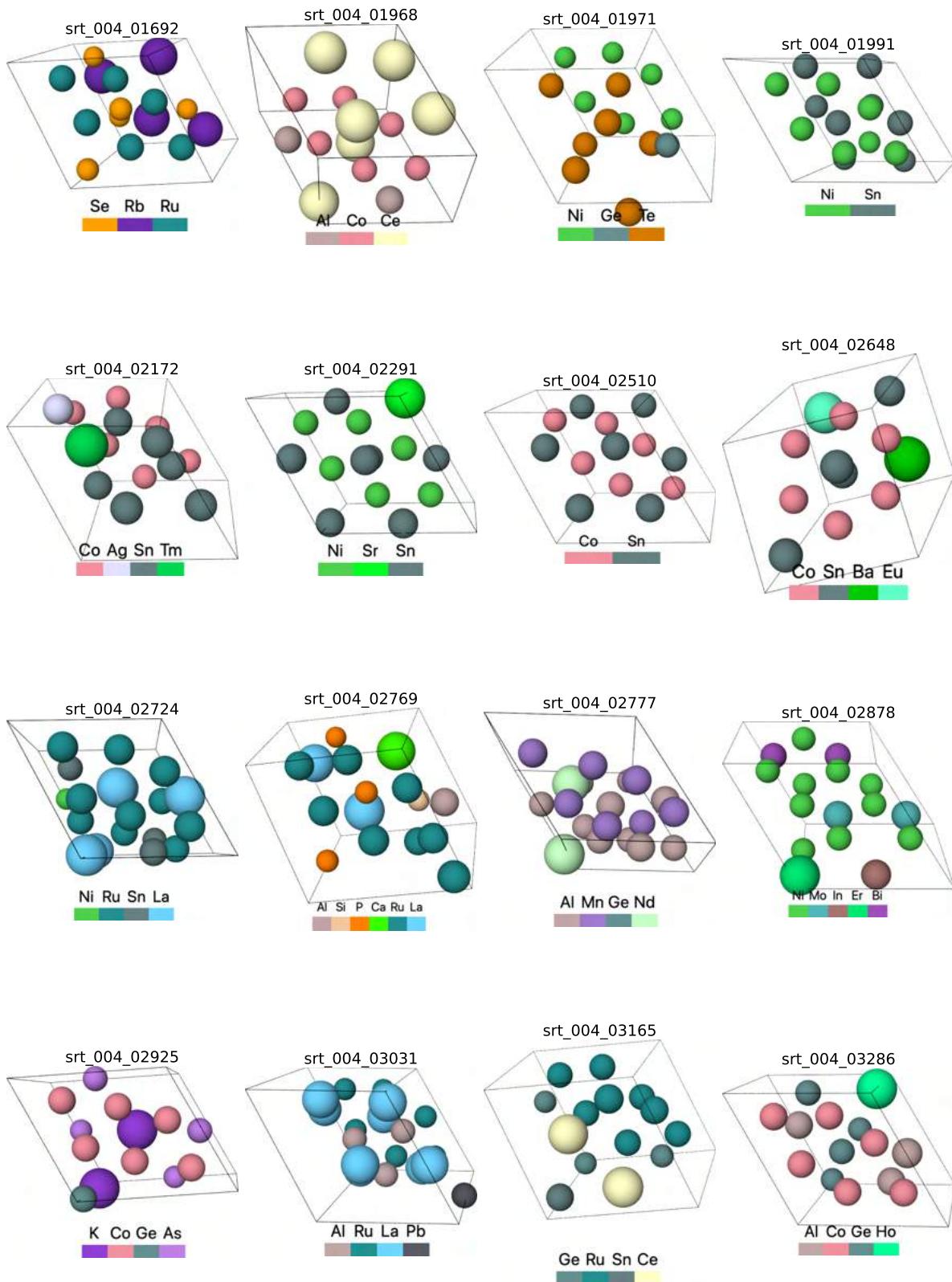


Figure S177. Generated materials with Small rhombitrihexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

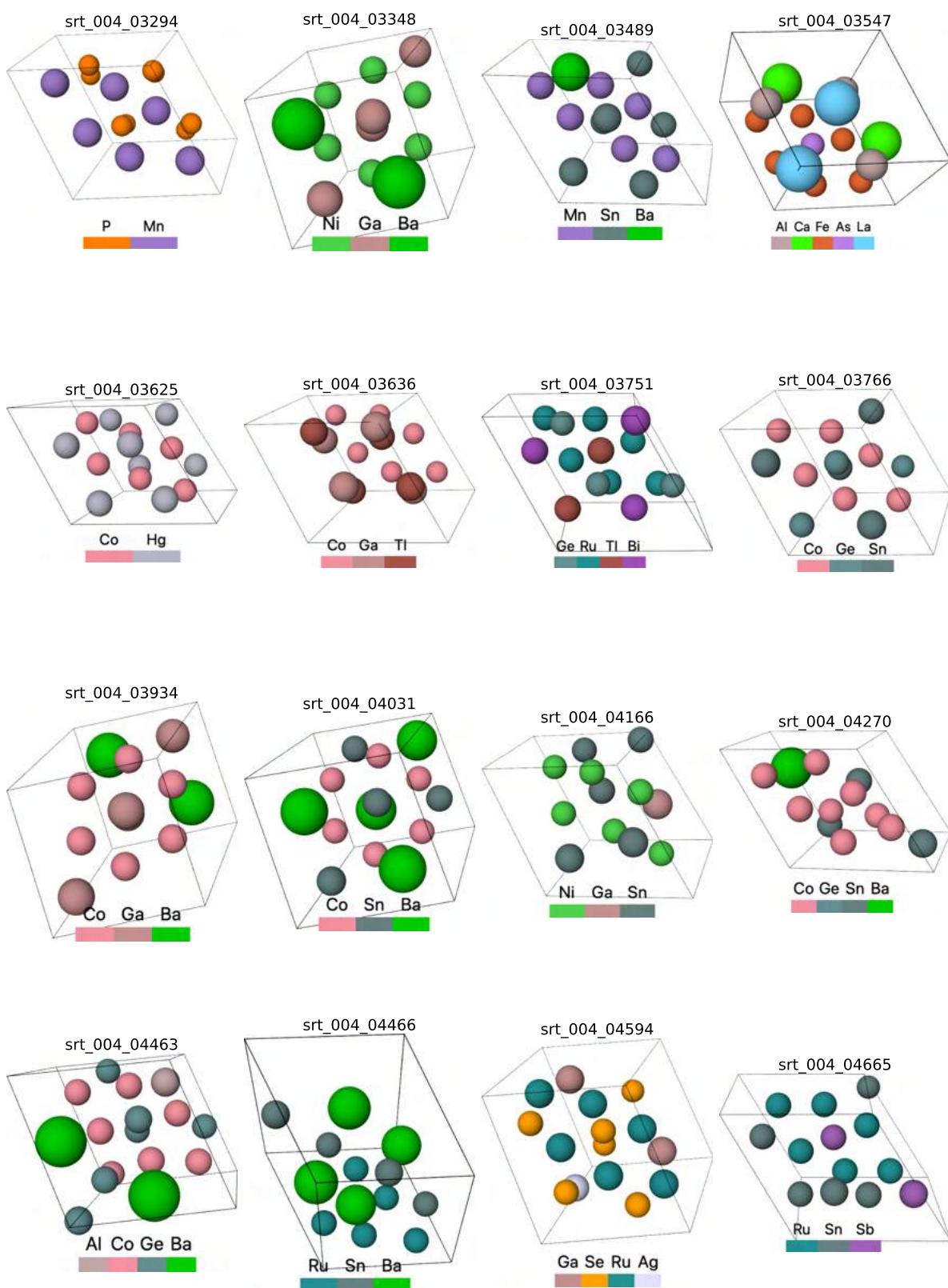


Figure S178. Generated materials with Small rhombitrihexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

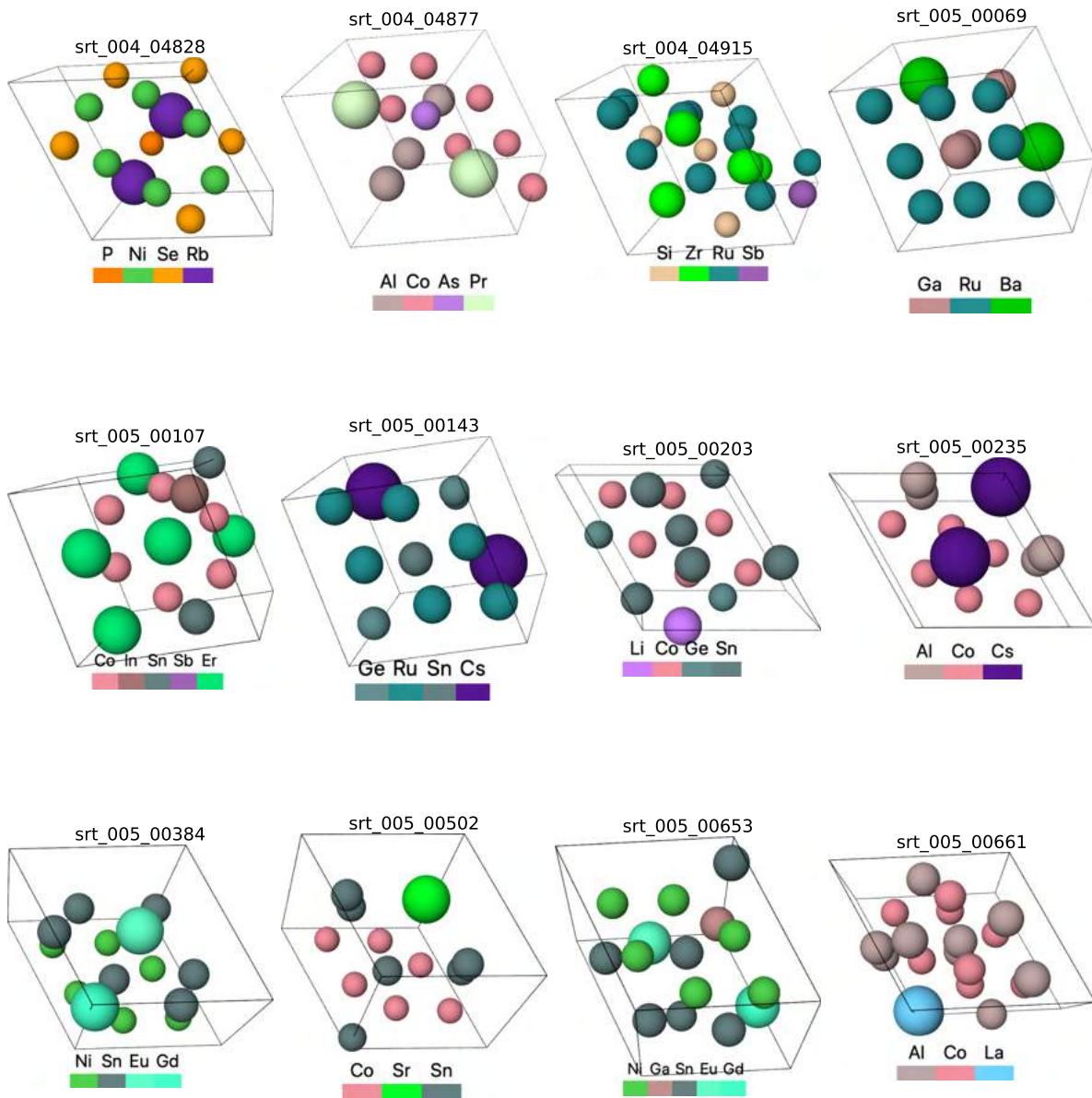


Figure S179. Generated materials with Small rhombitrihexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

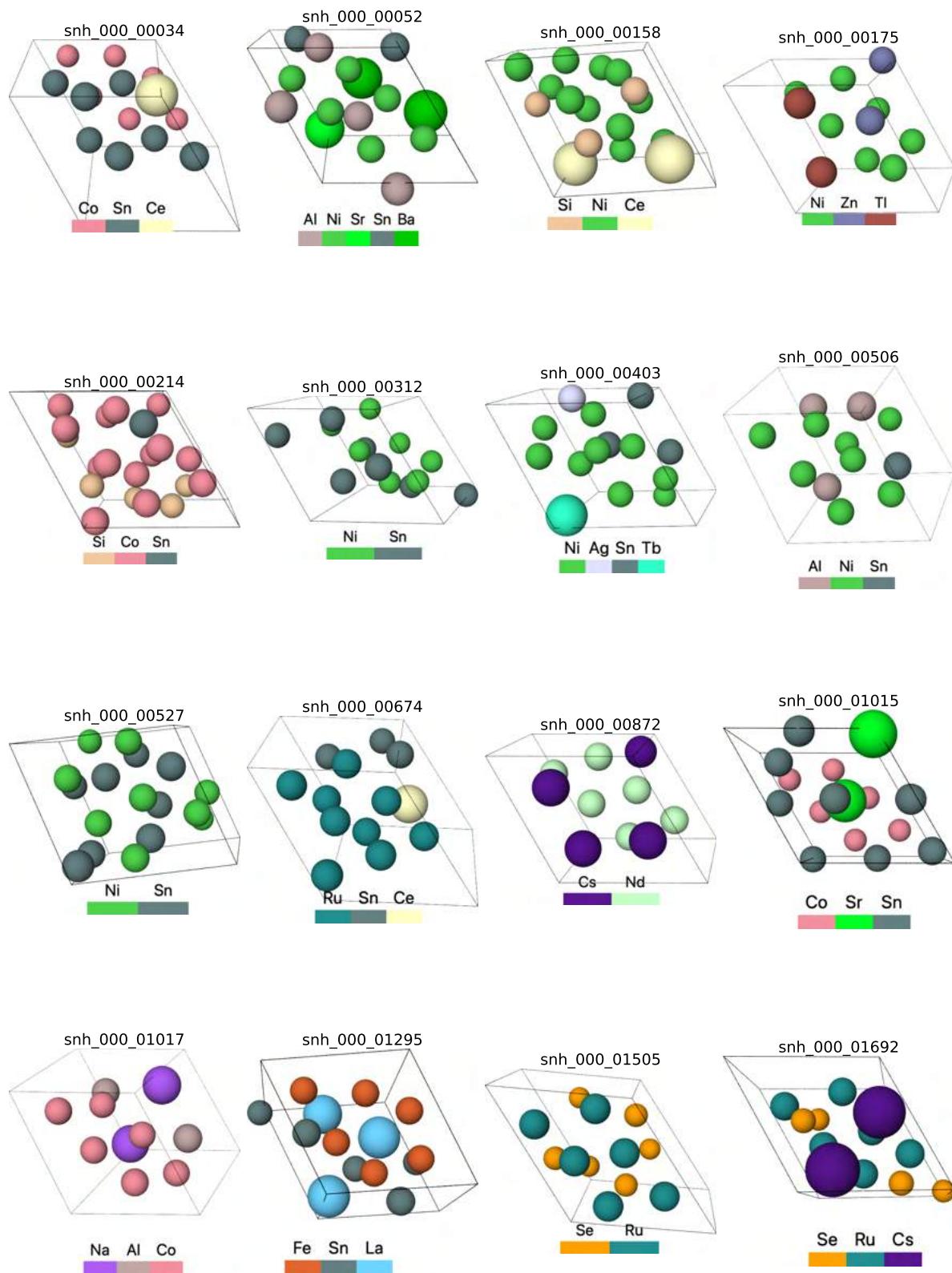


Figure S180. Generated materials with Snub hexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

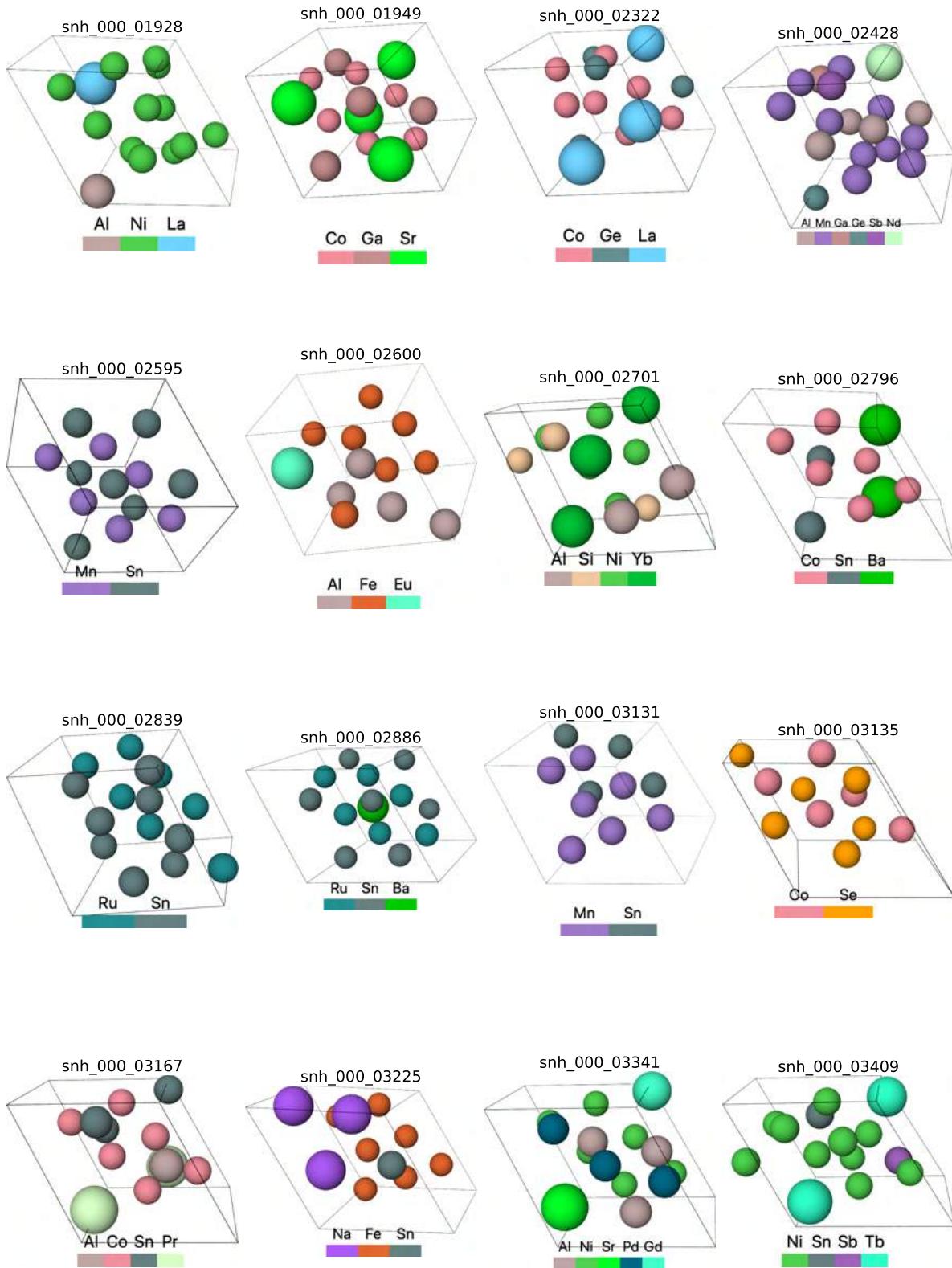


Figure S181. Generated materials with Snub hexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

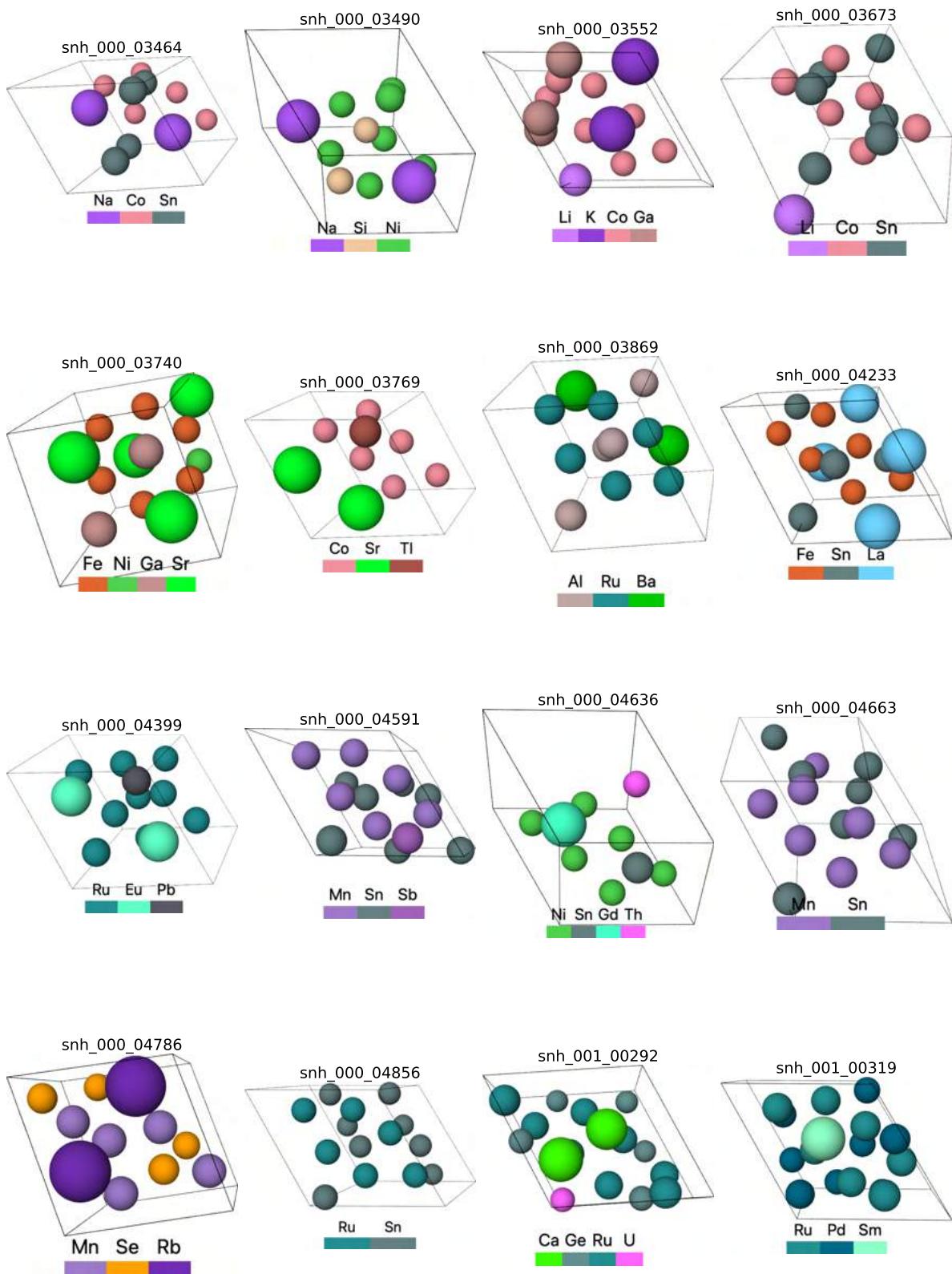


Figure S182. Generated materials with Snub hexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

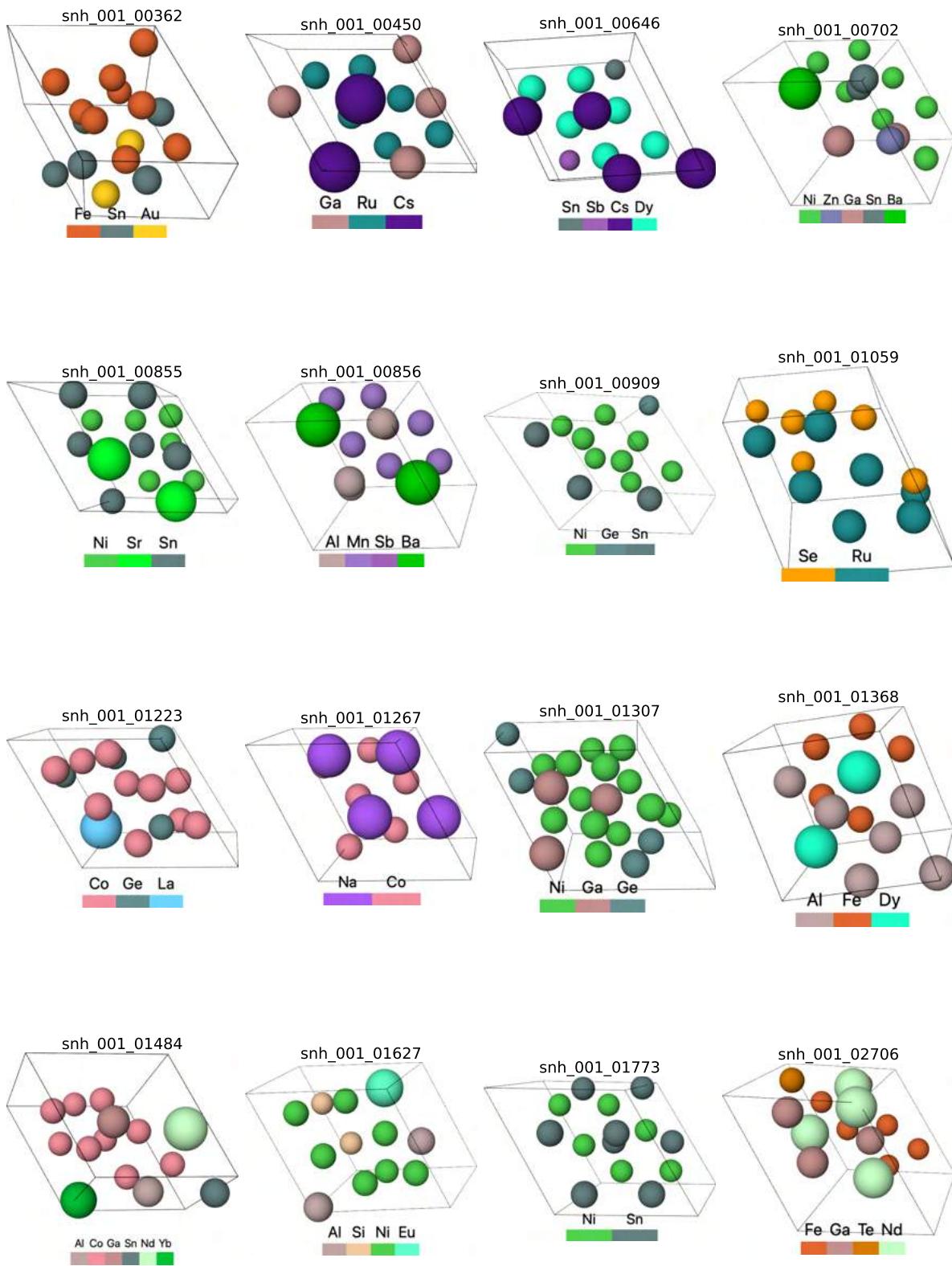


Figure S183. Generated materials with Snub hexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

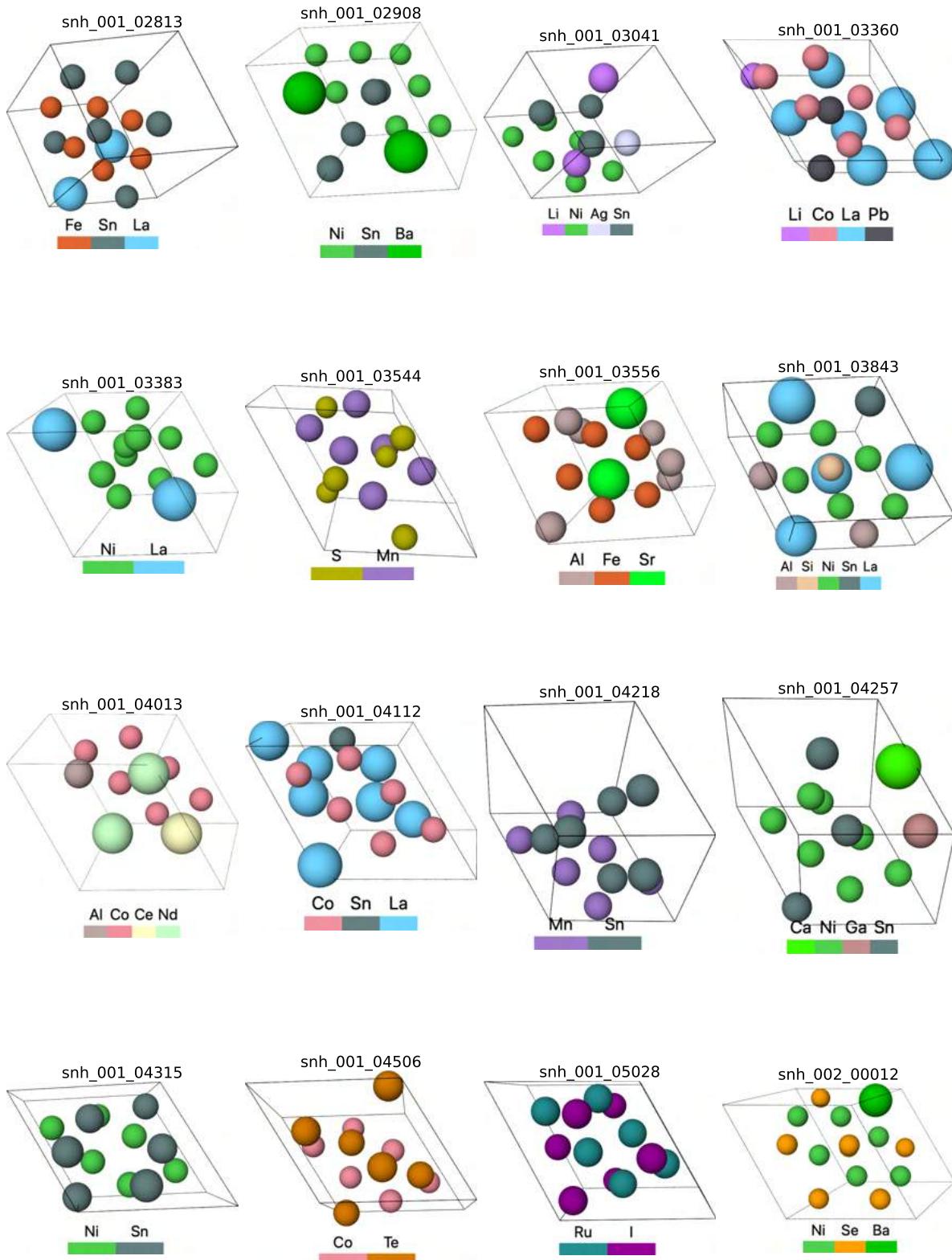


Figure S184. Generated materials with Snub hexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

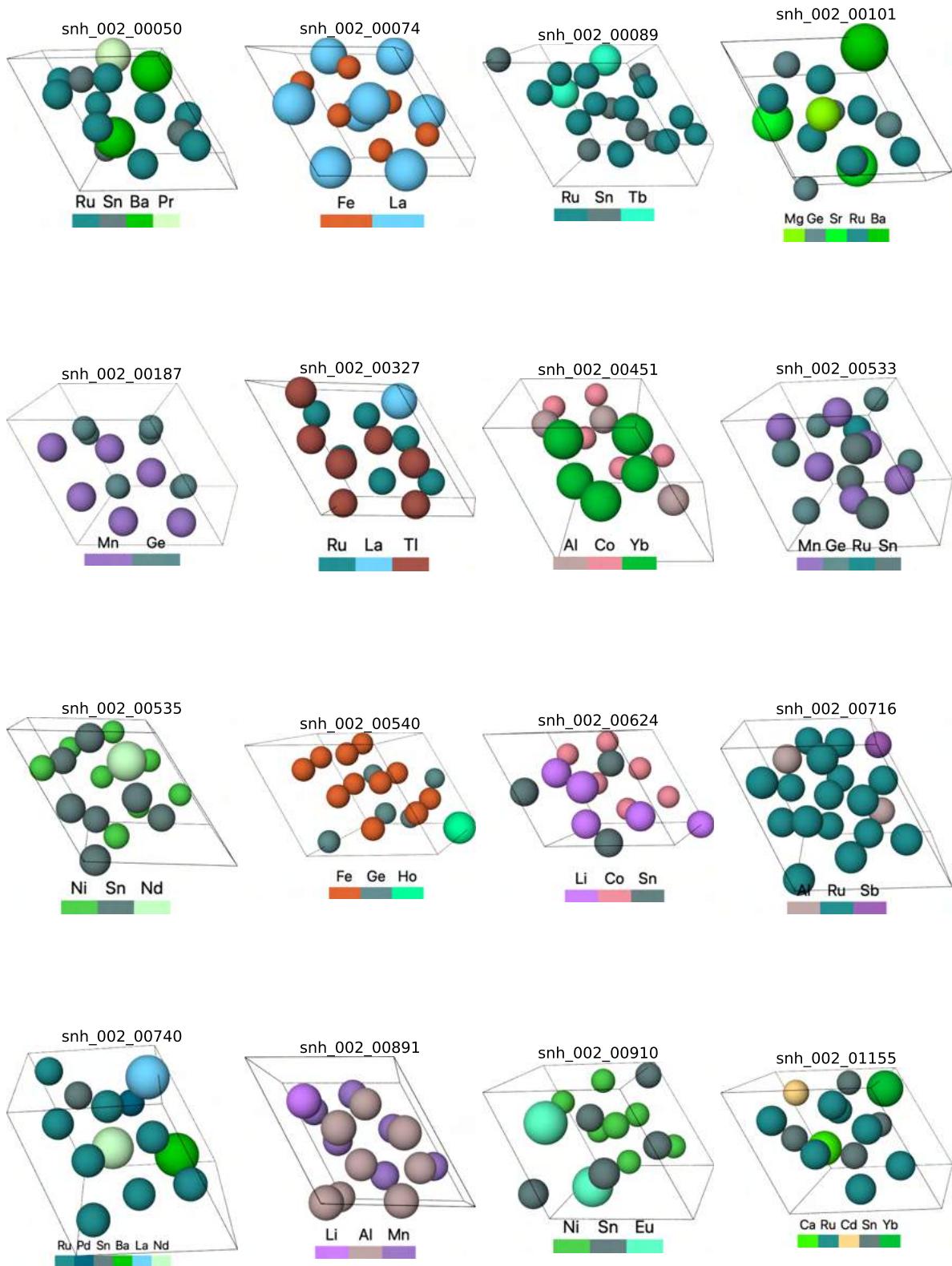


Figure S185. Generated materials with Snub hexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

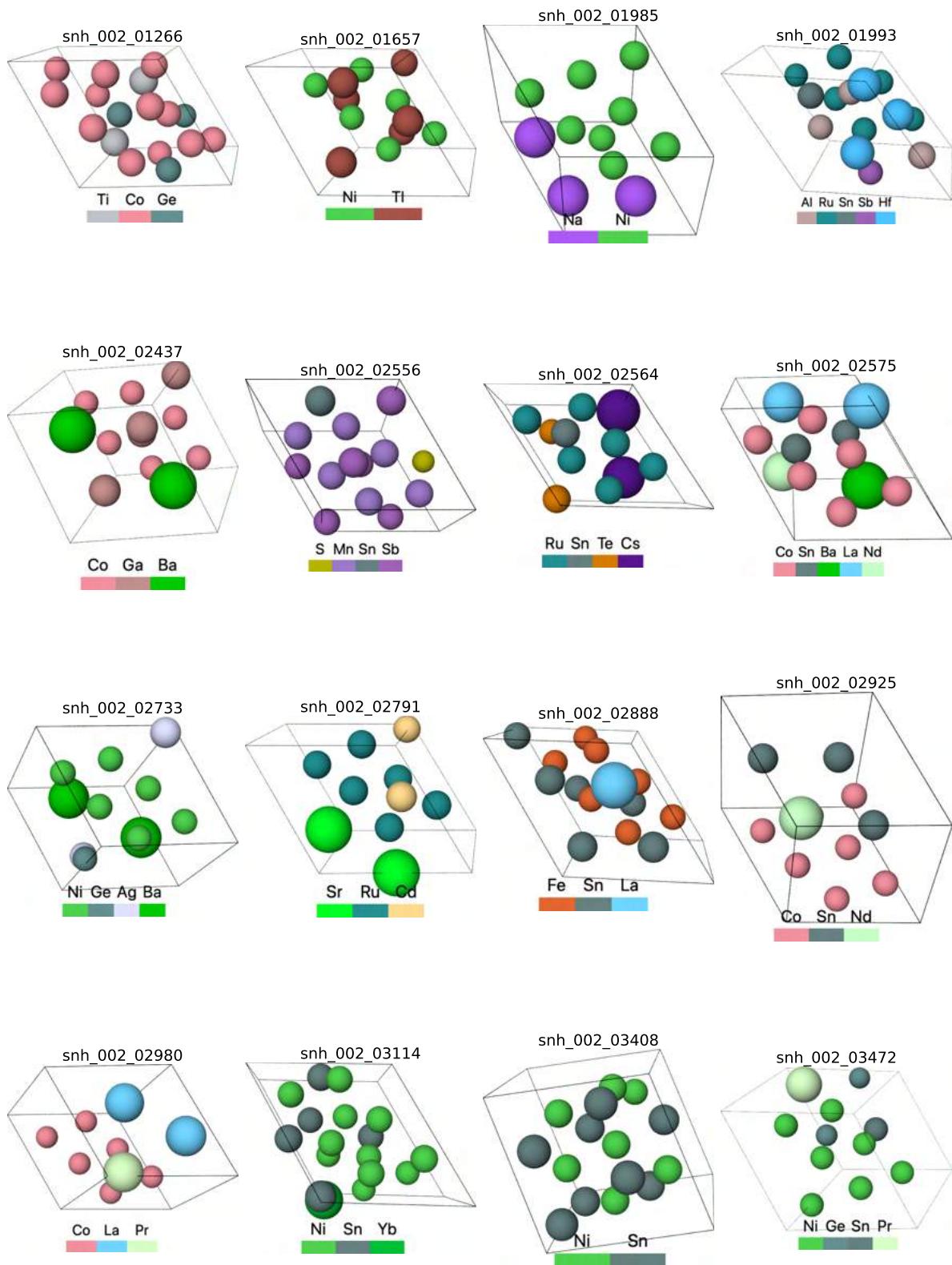


Figure S186. Generated materials with Snub hexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

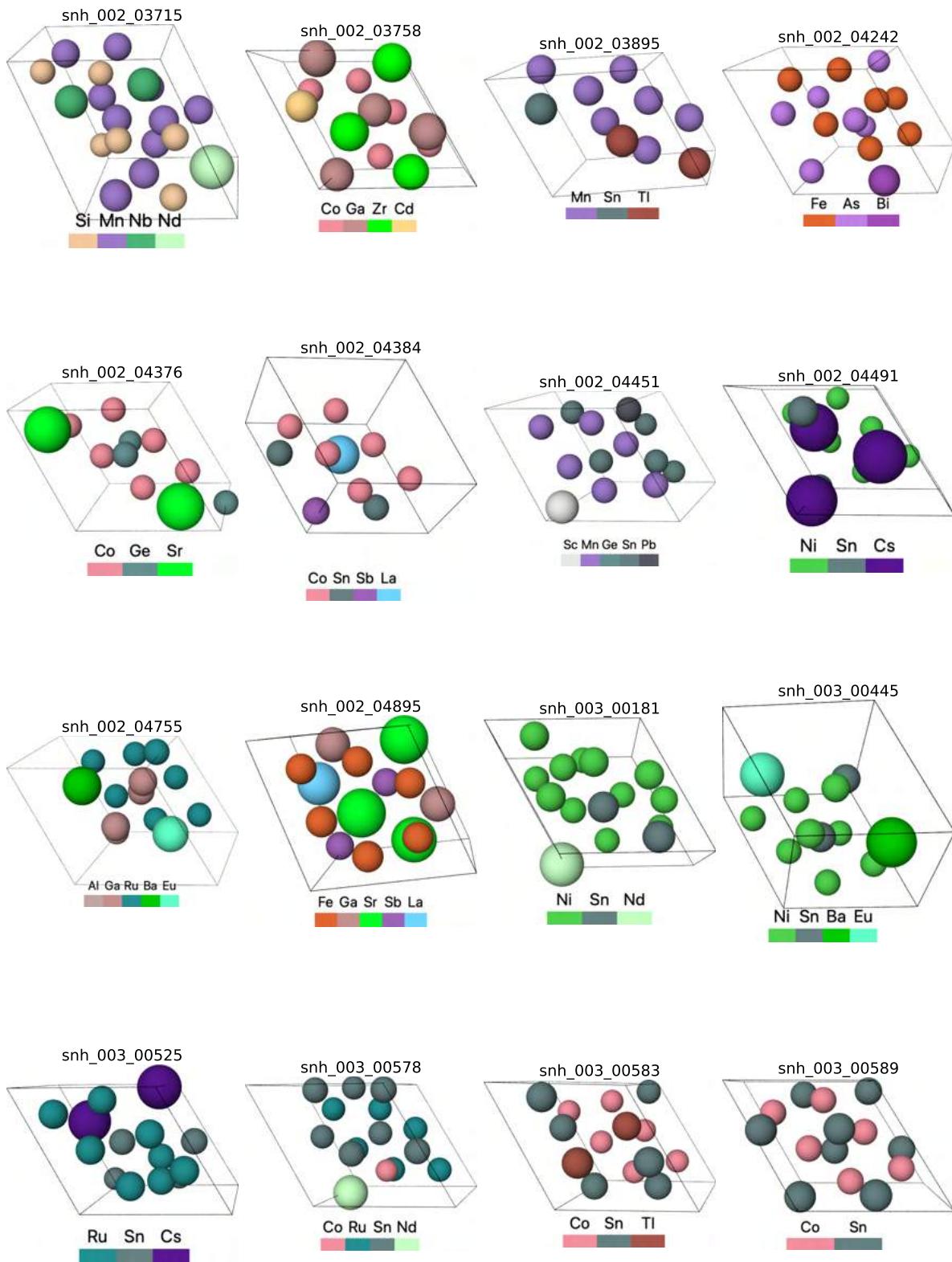


Figure S187. Generated materials with Snub hexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

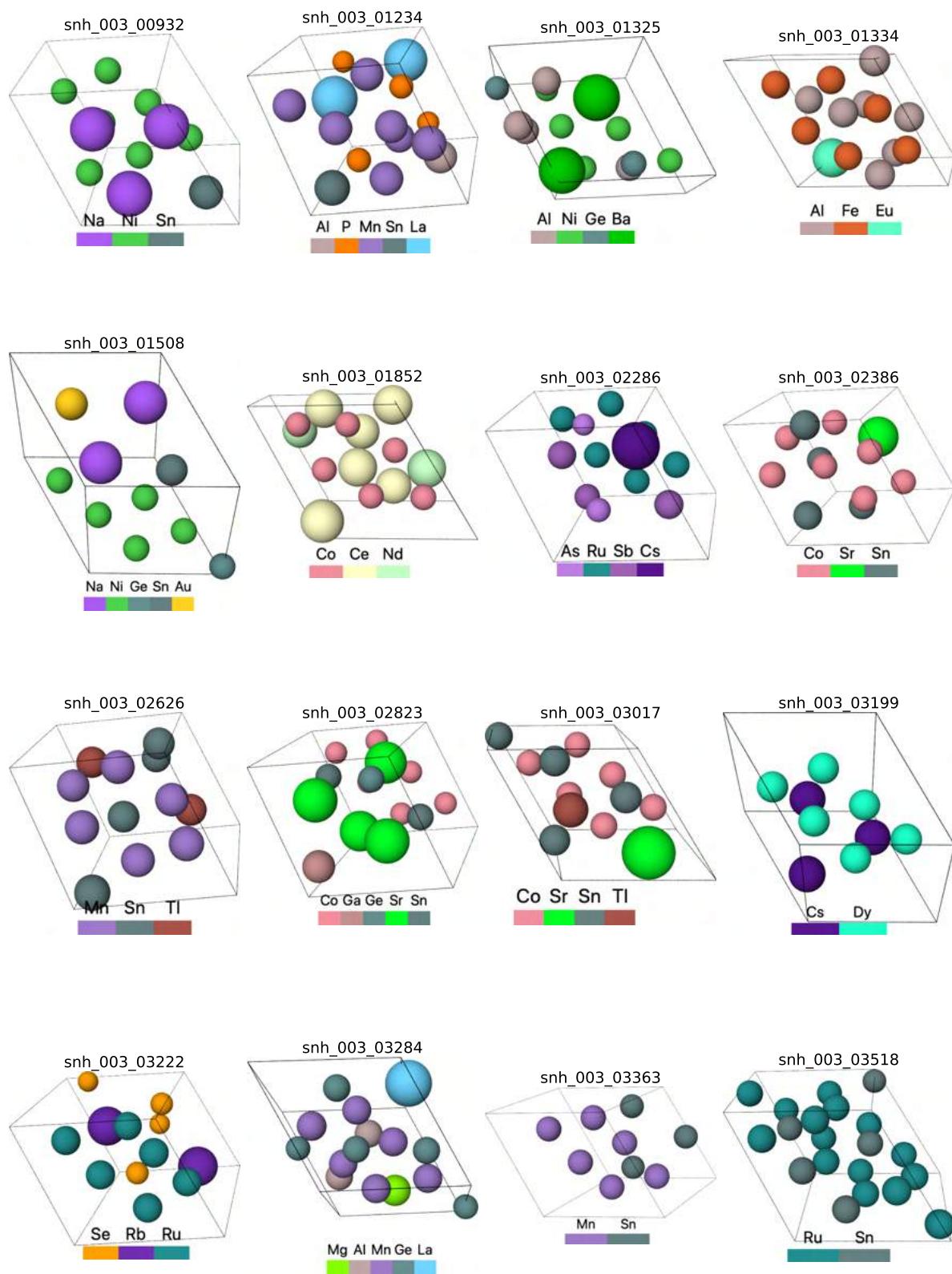


Figure S188. Generated materials with Snub hexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

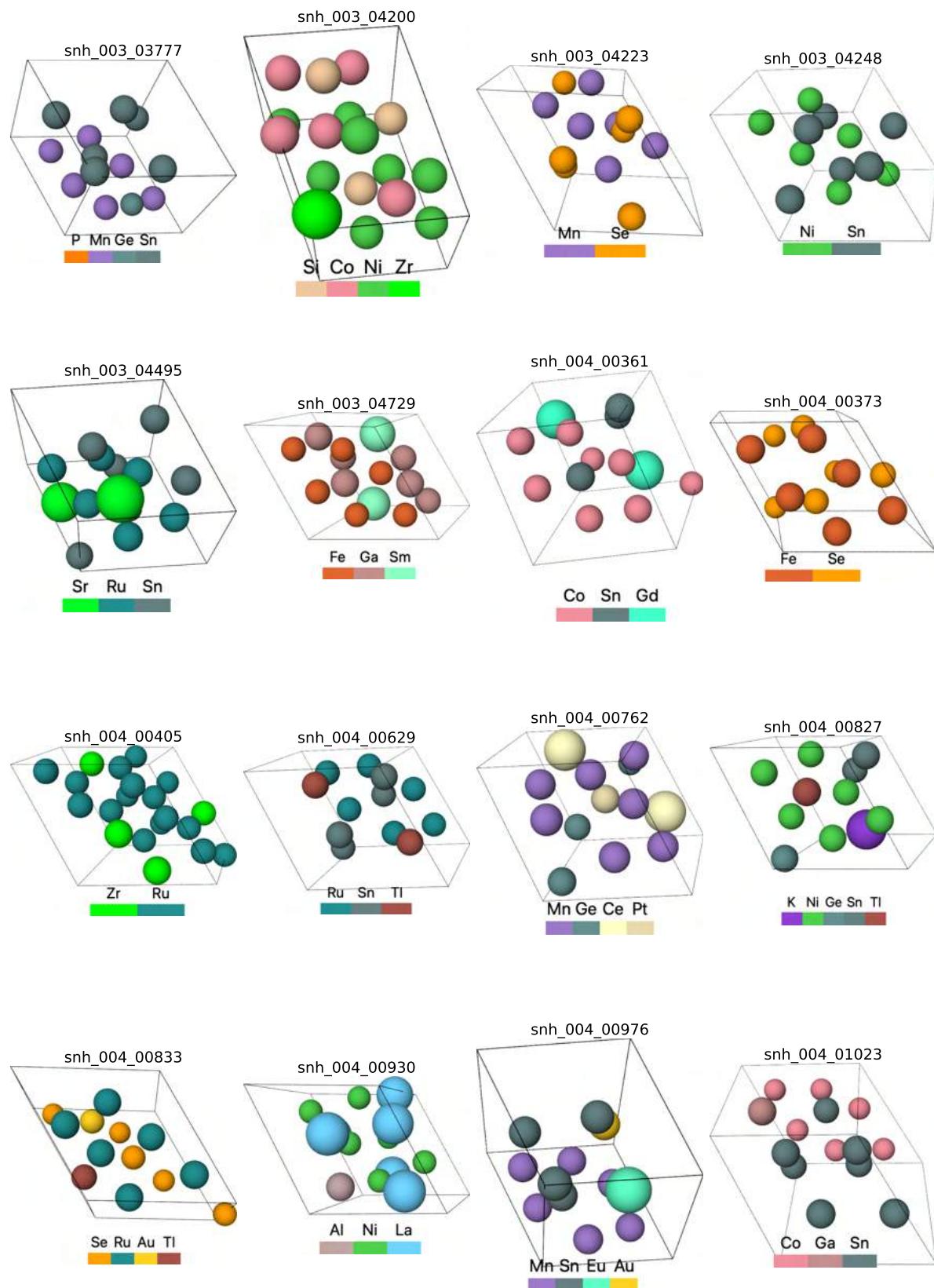


Figure S189. Generated materials with Snub hexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

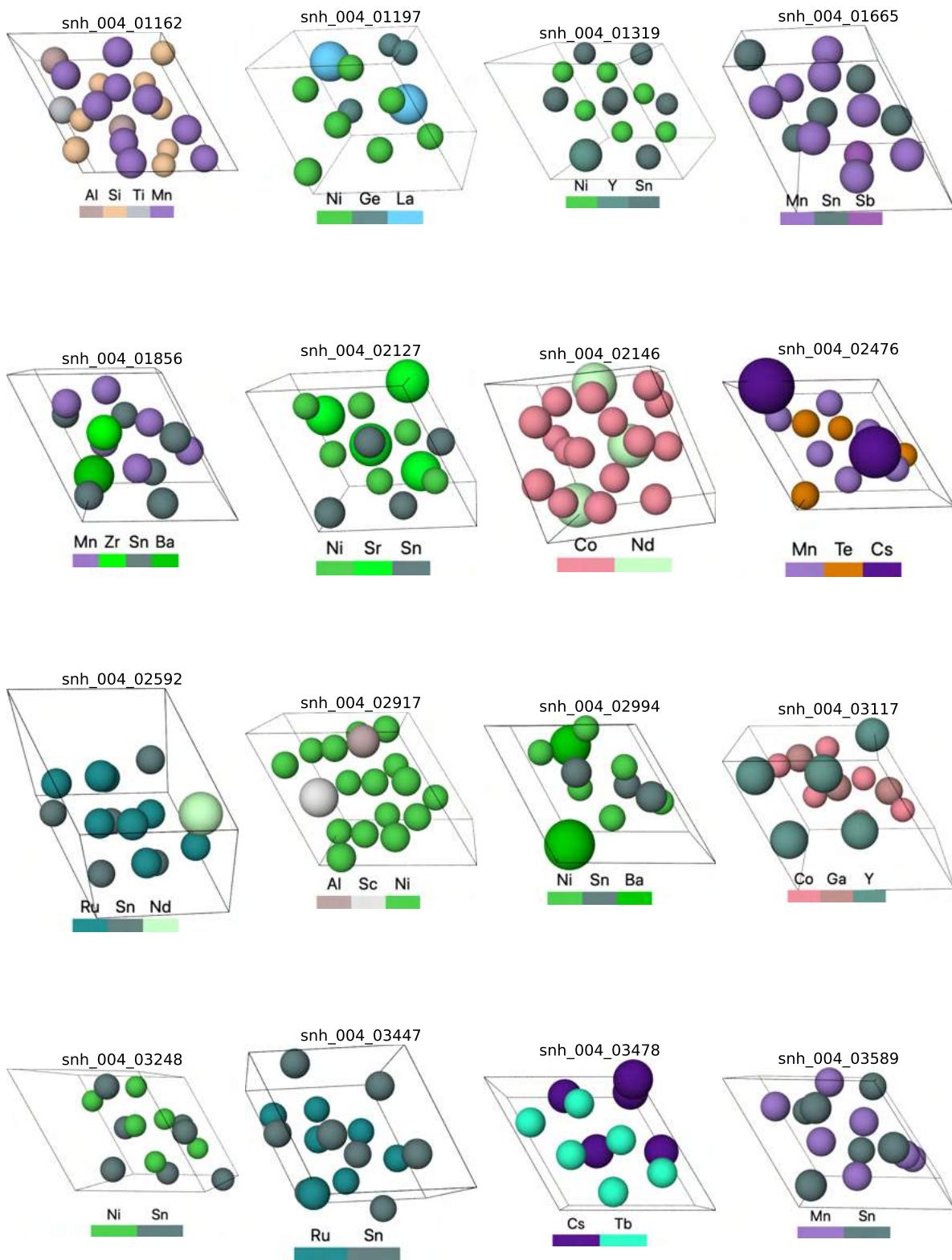


Figure S190. Generated materials with Snub hexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

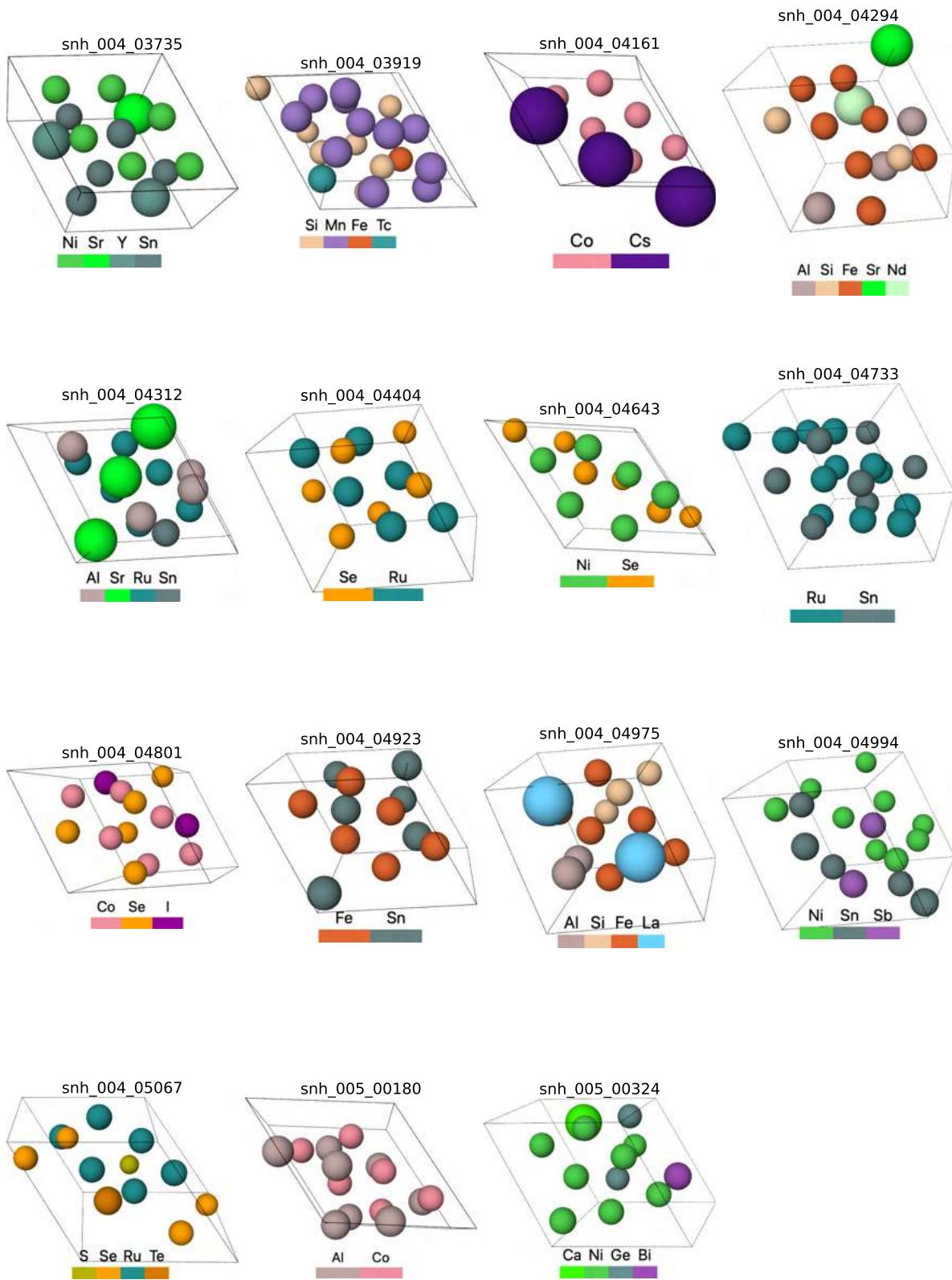


Figure S191. Generated materials with Snub hexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 2.0 \text{ \AA}$, and $d_{xy} = 1.0 \text{ \AA}$ as the thresholds.

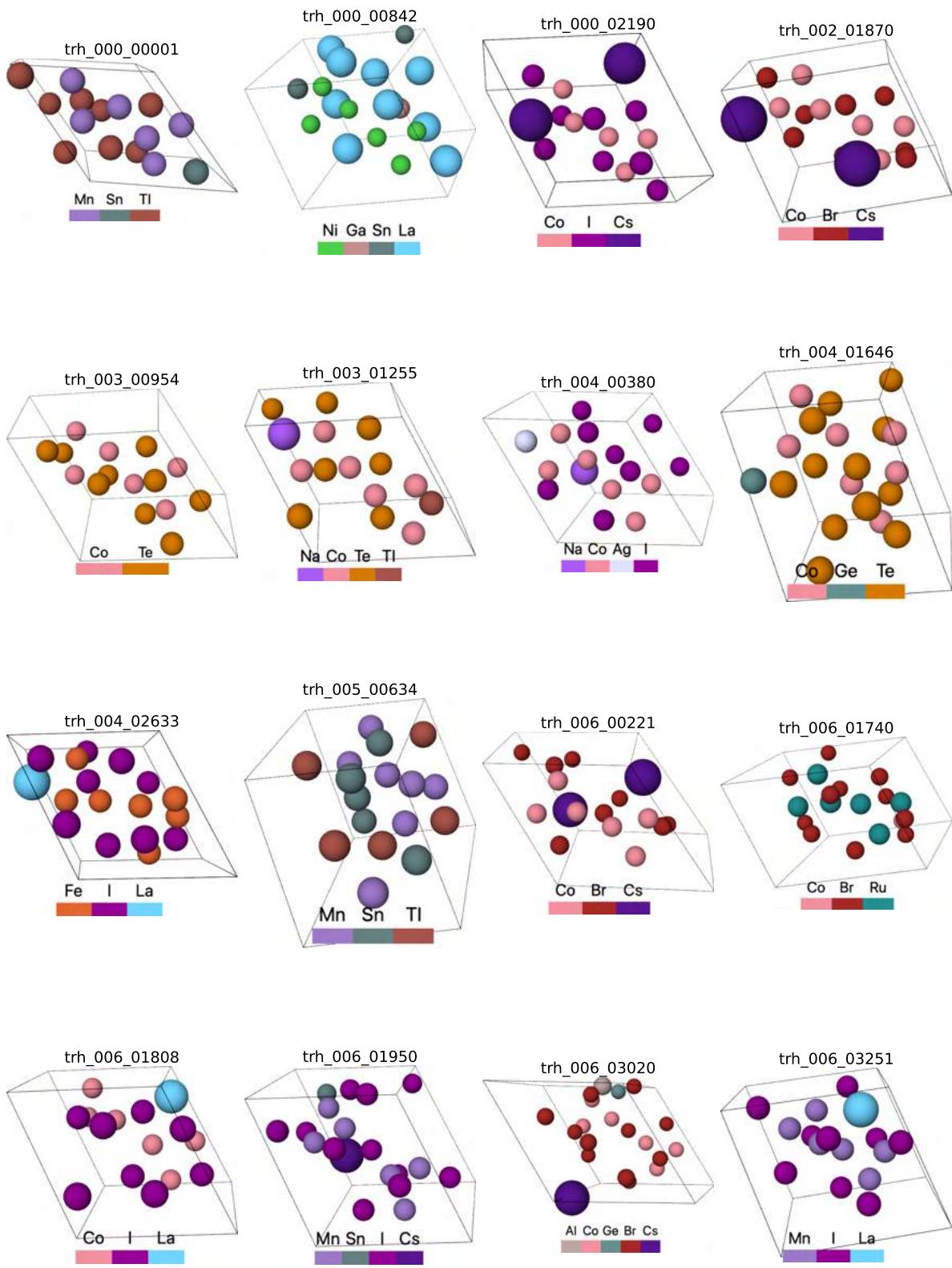


Figure S192. Generated materials with Truncated hexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 3.0 \text{ \AA}$, and $d_{xy} = 1.5 \text{ \AA}$ as the thresholds.

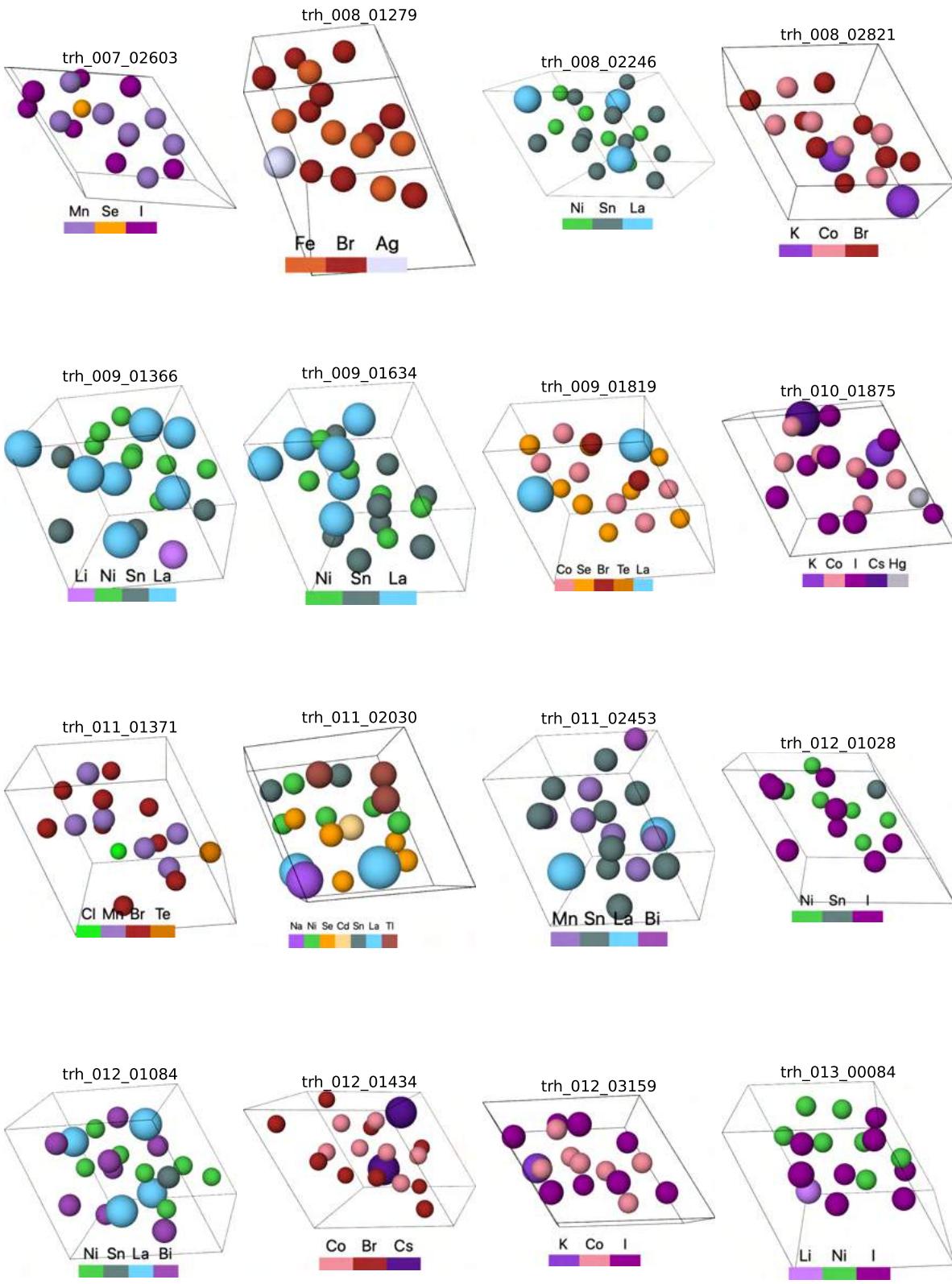


Figure S193. Generated materials with Truncated hexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 3.0 \text{ \AA}$, and $d_{xy} = 1.5 \text{ \AA}$ as the thresholds.

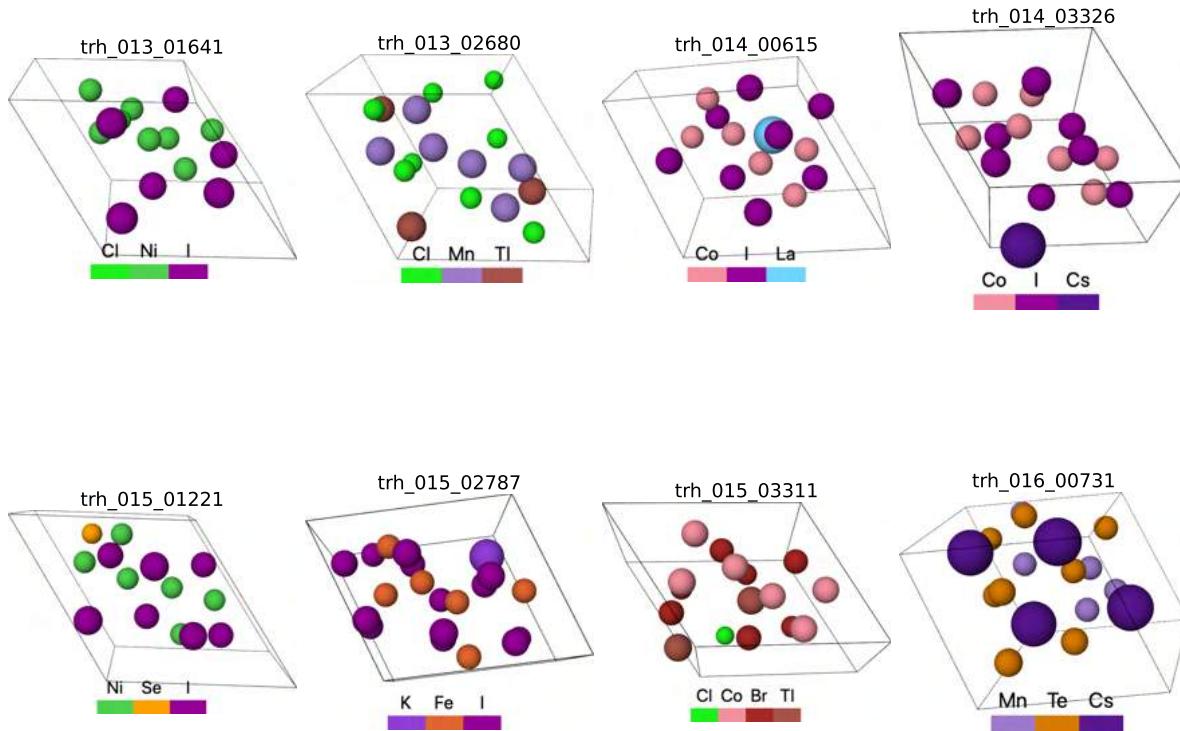


Figure S194. Generated materials with Truncated hexagonal lattice structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 3.0 \text{ \AA}$, and $d_{xy} = 1.5 \text{ \AA}$ as the thresholds.

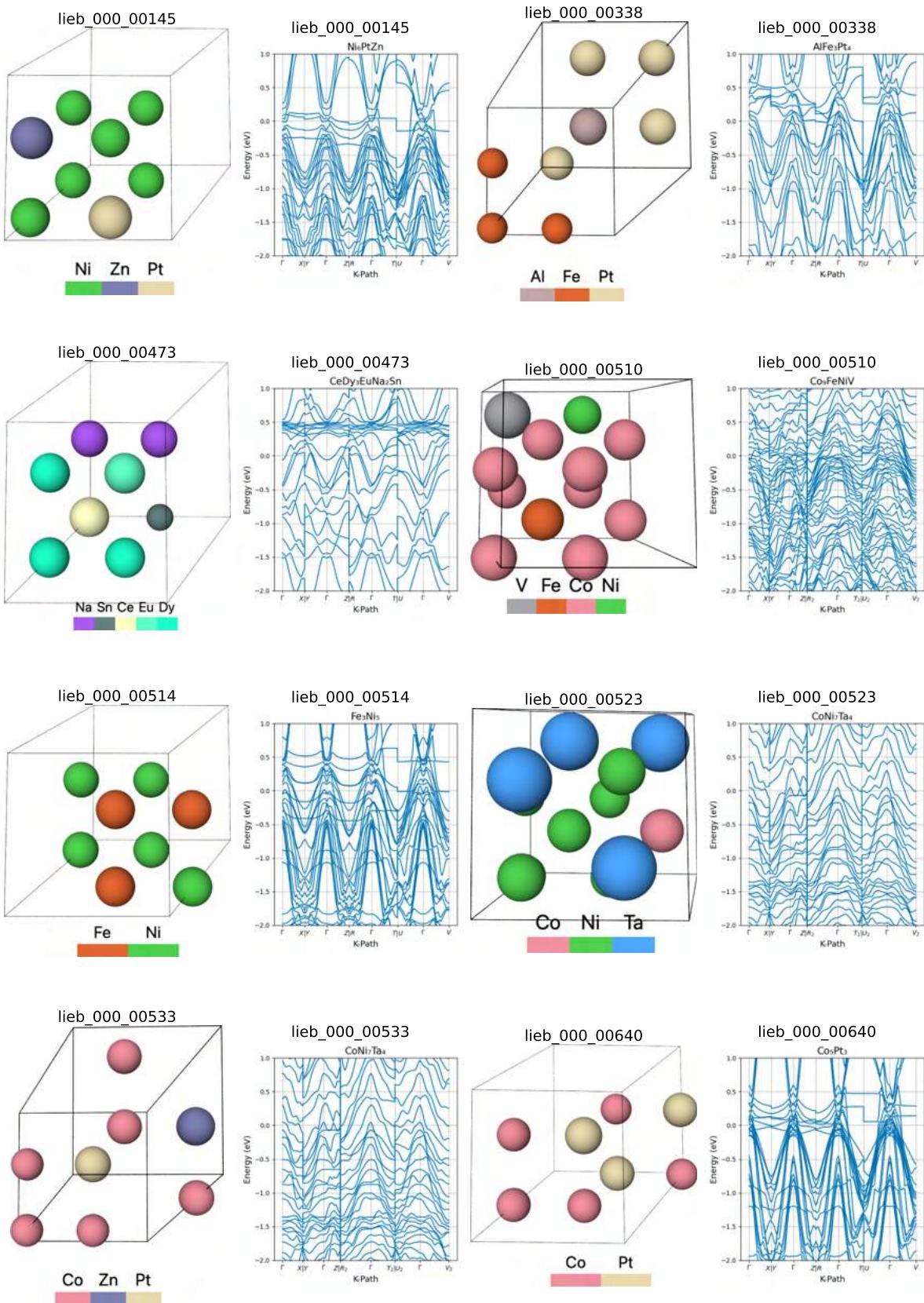


Figure S195. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

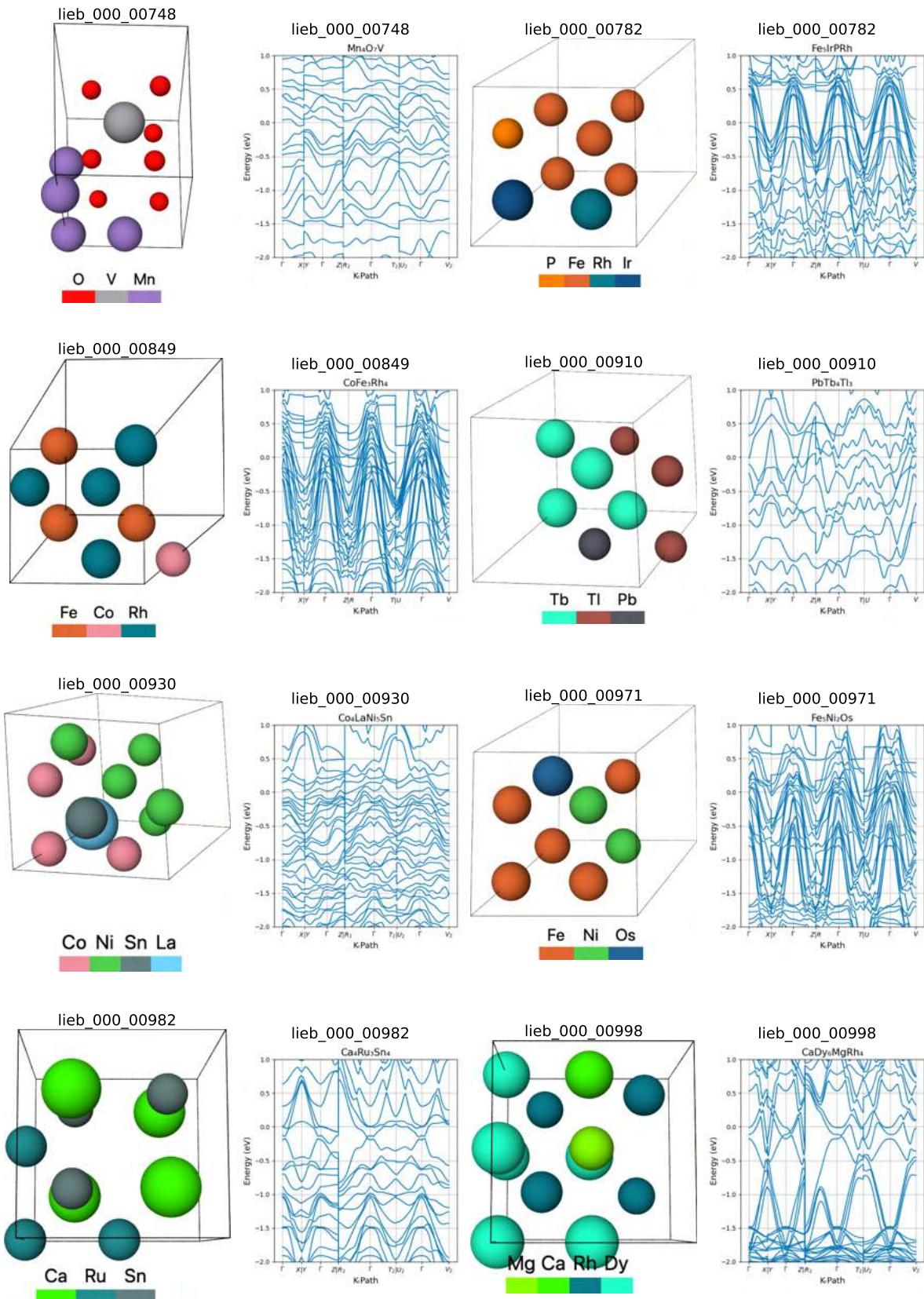


Figure S196. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

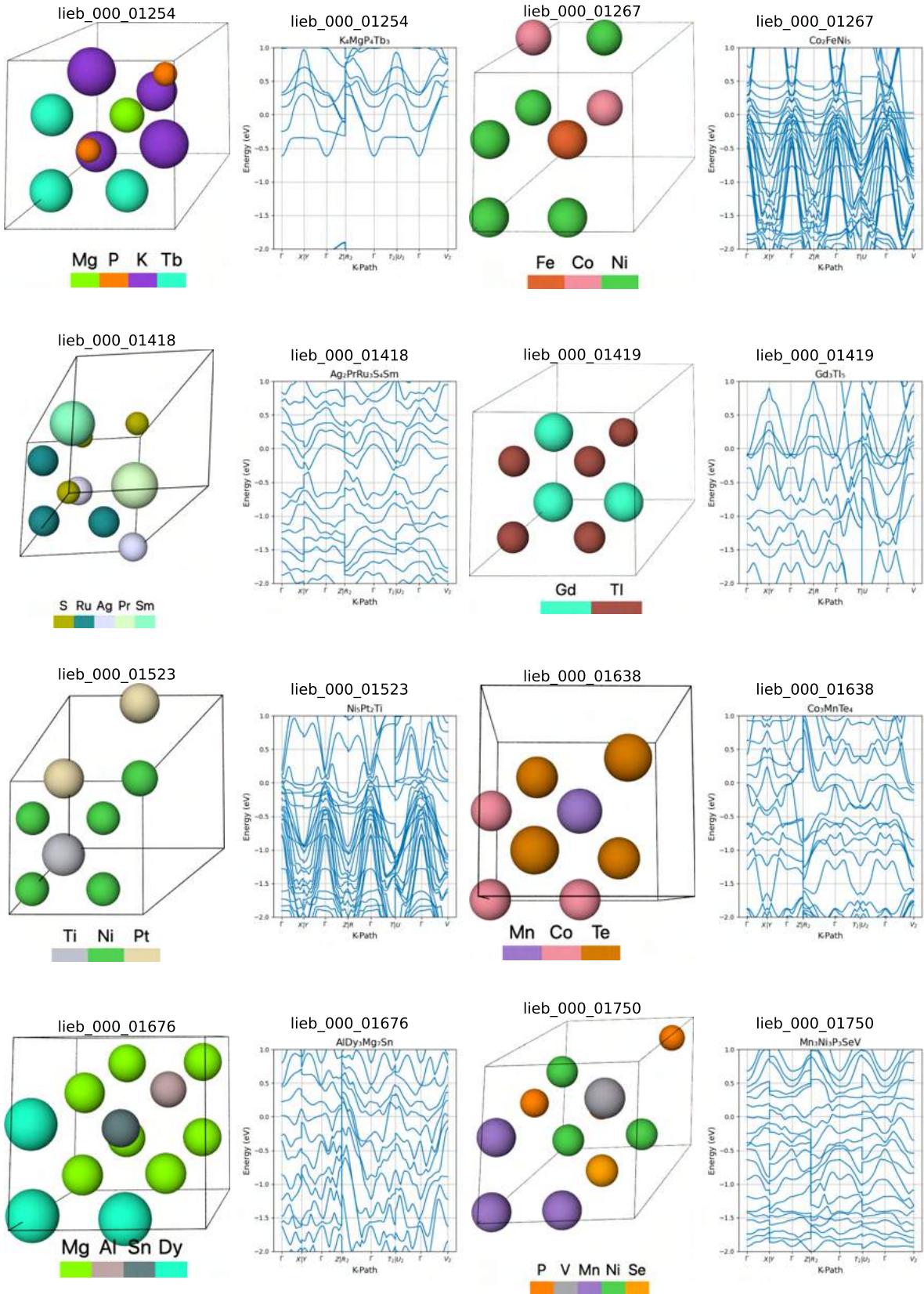


Figure S197. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

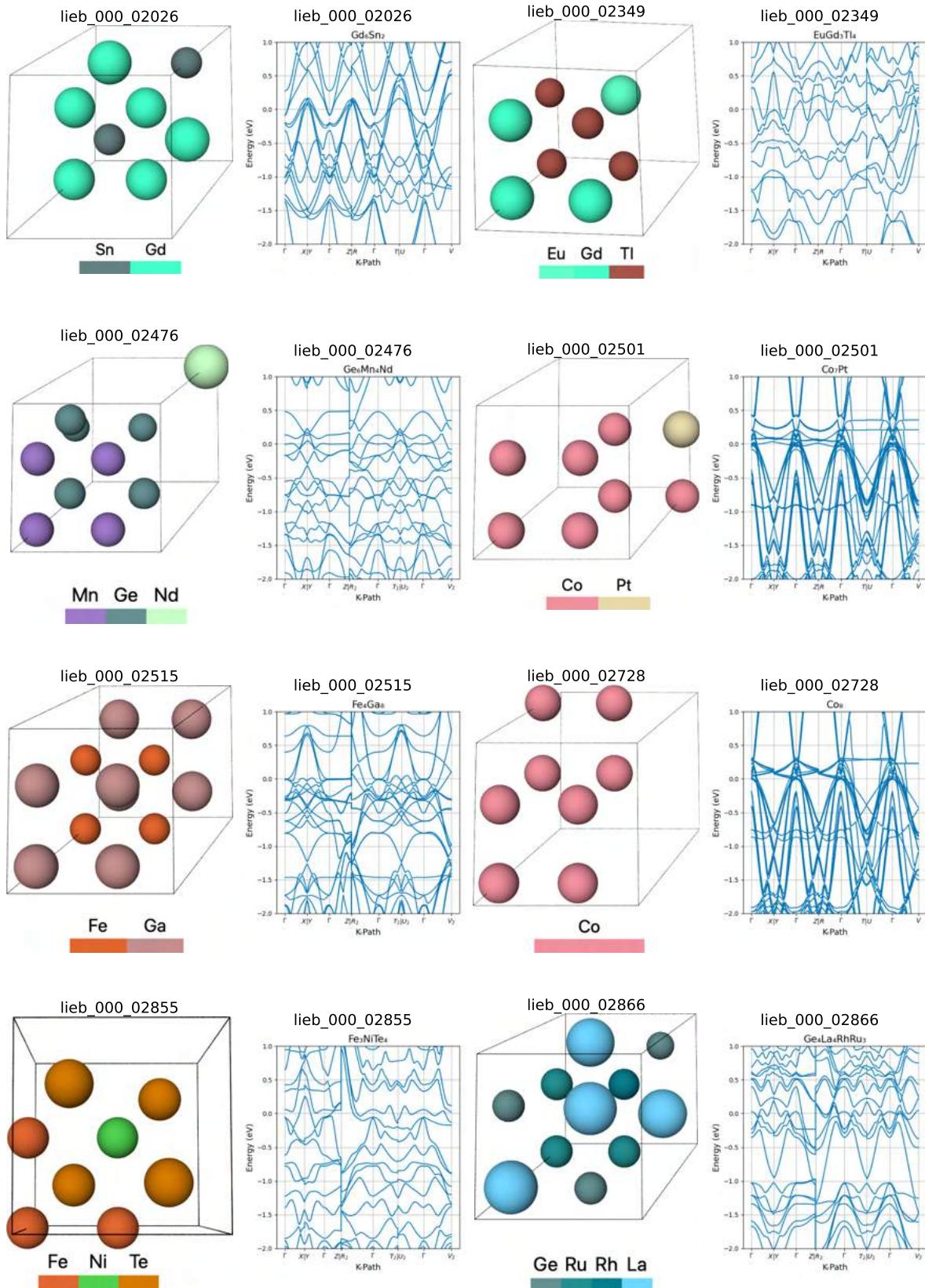


Figure S198. Generated materials with Lieb lattice structures and the corresponding band structures
We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

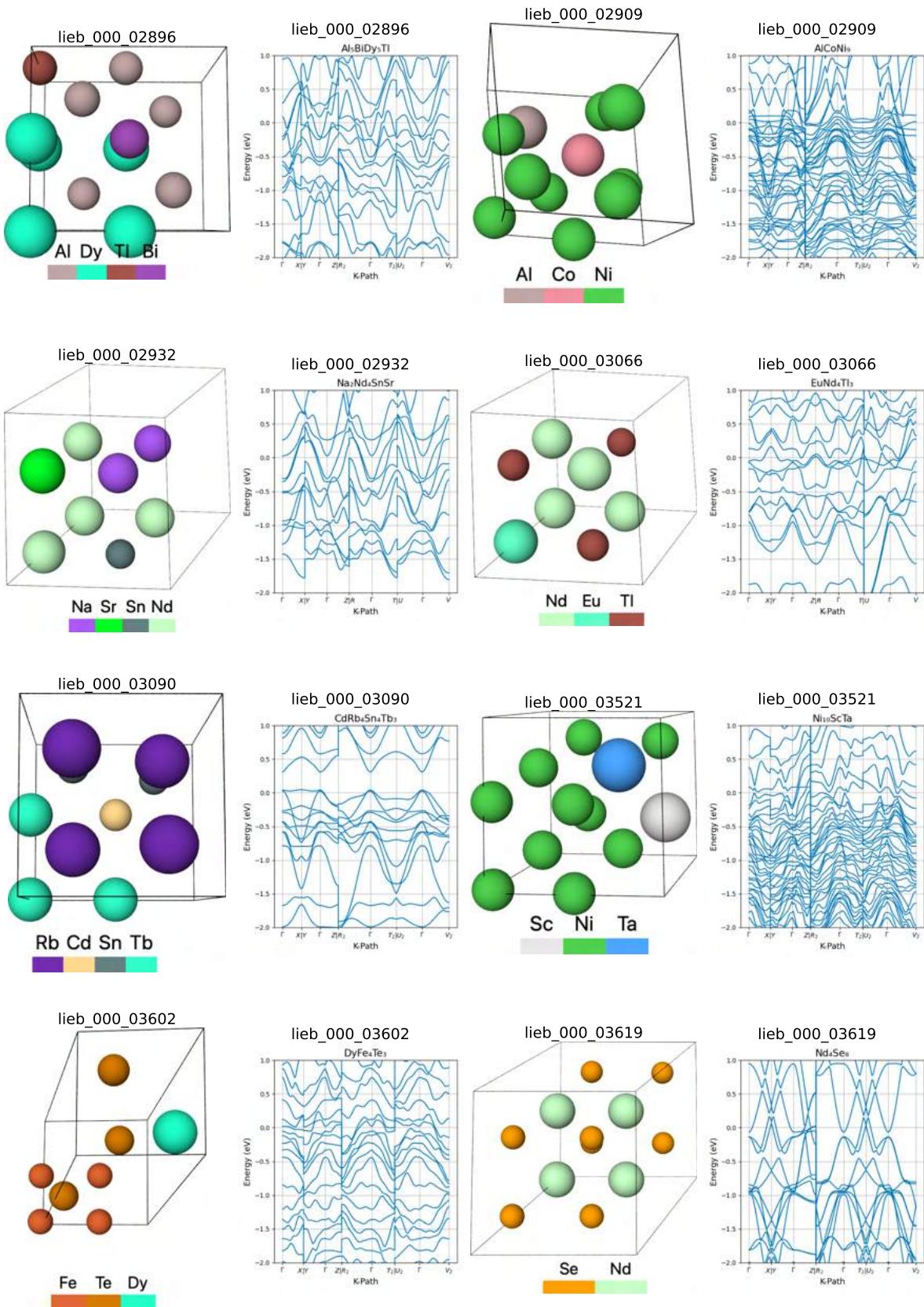


Figure S199. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

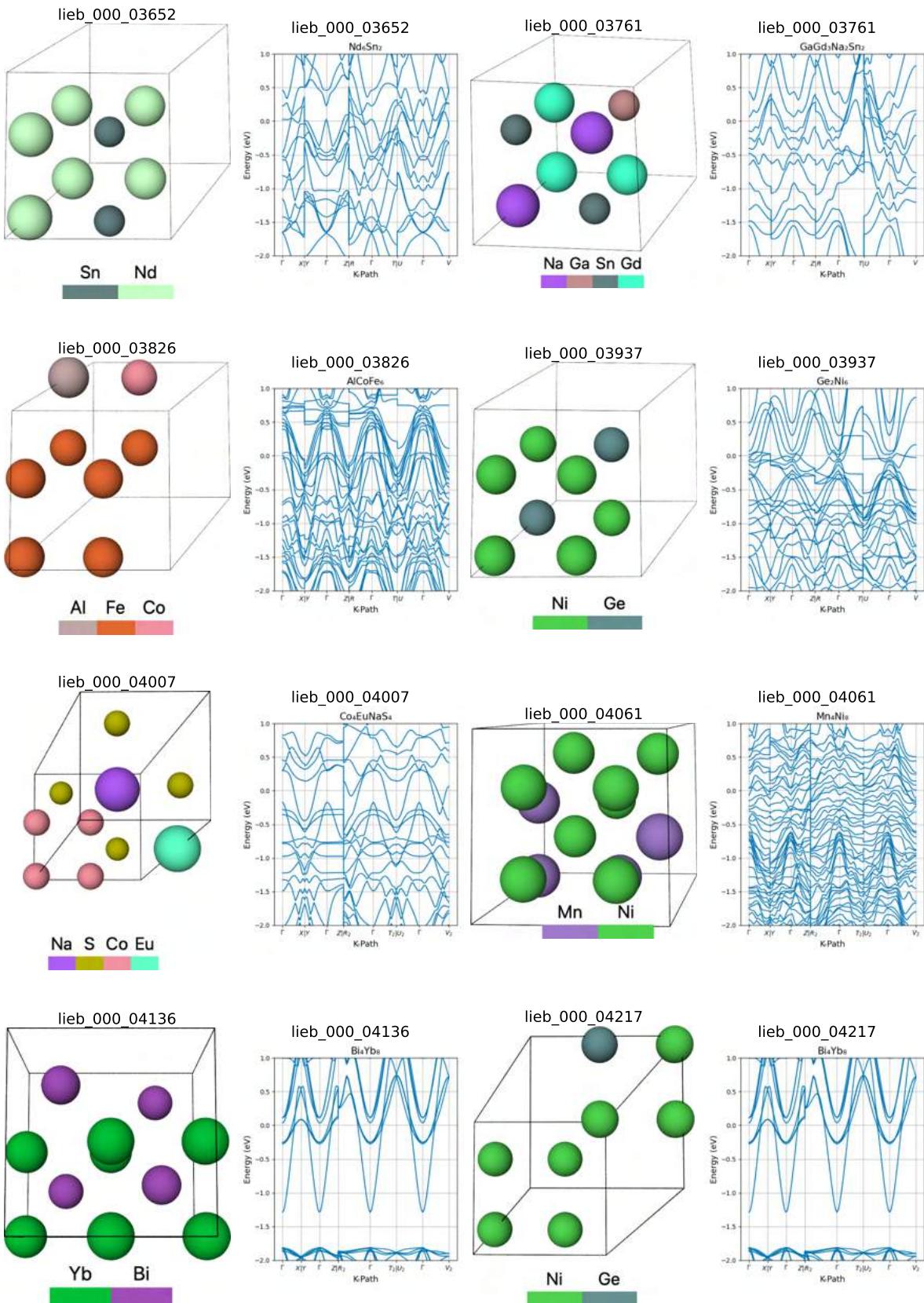


Figure S200. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

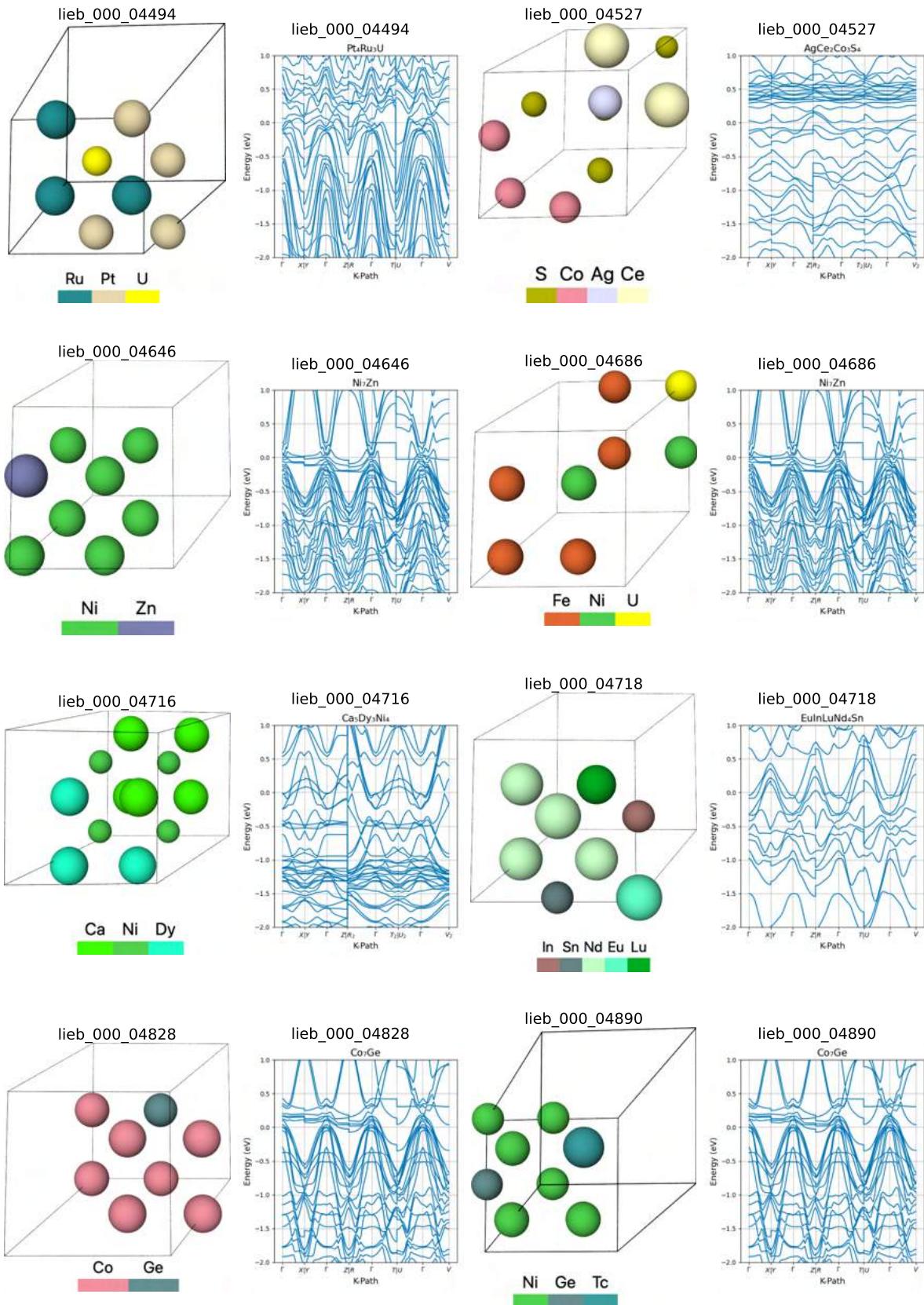


Figure S201. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

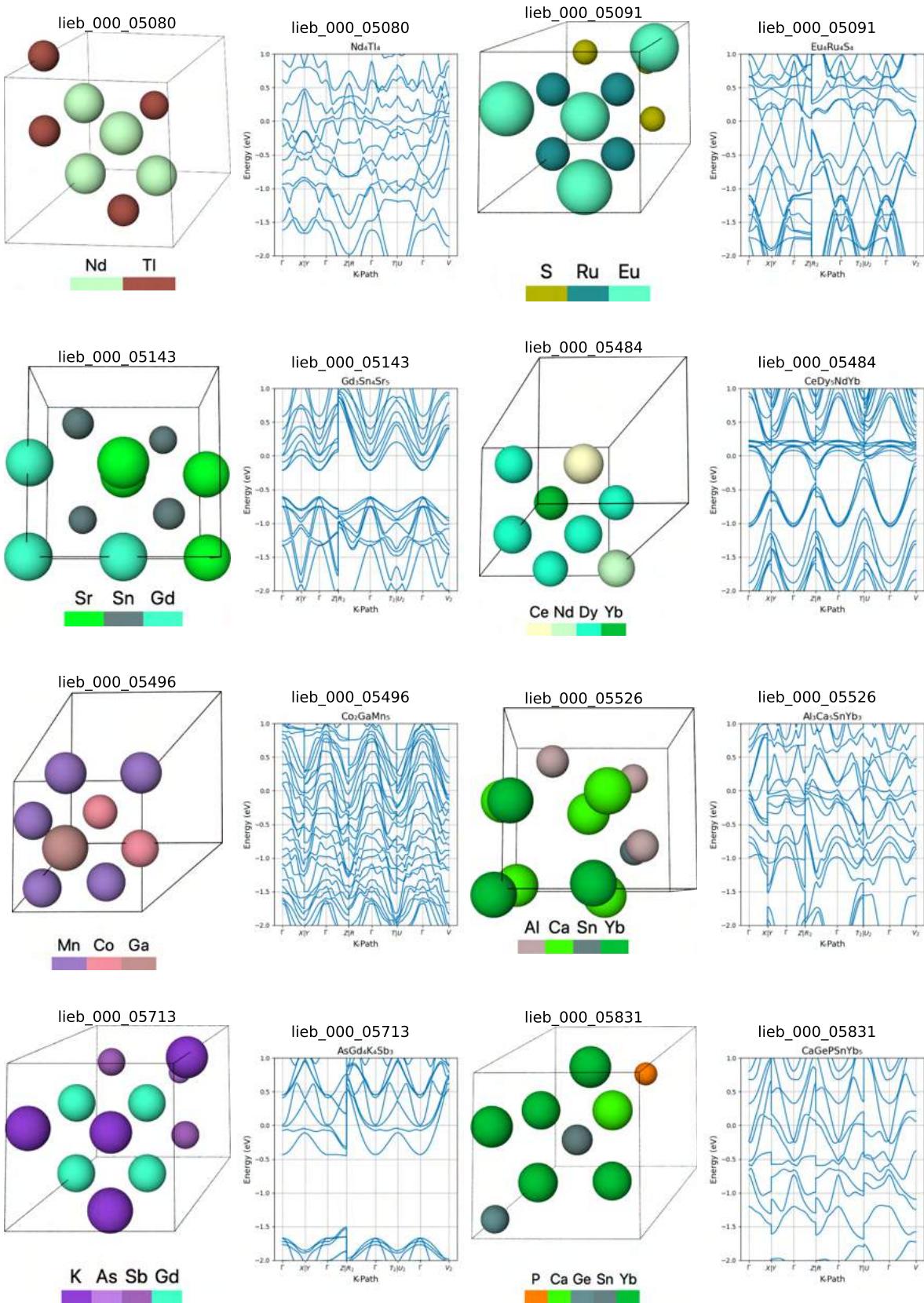


Figure S202. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

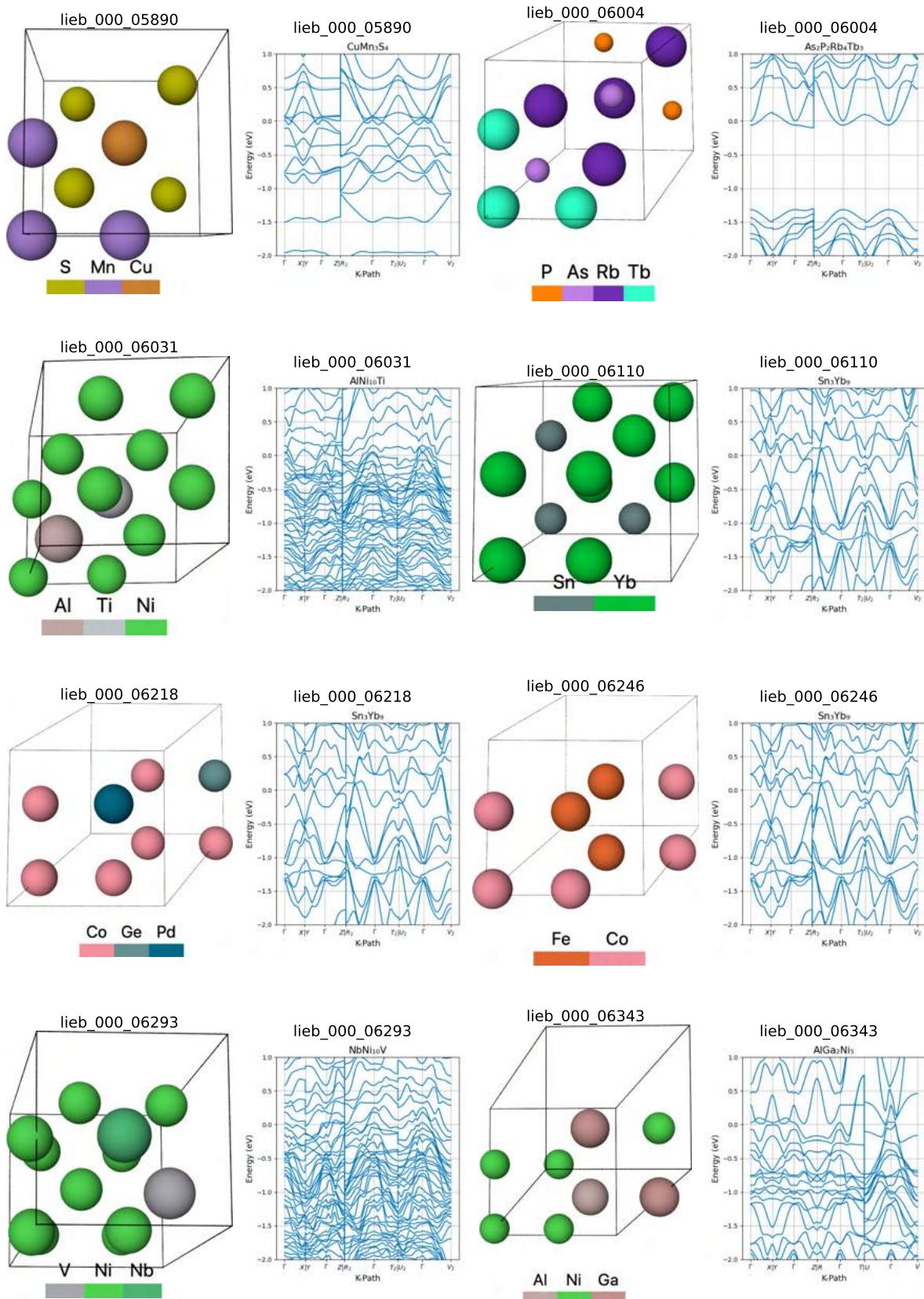


Figure S203. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

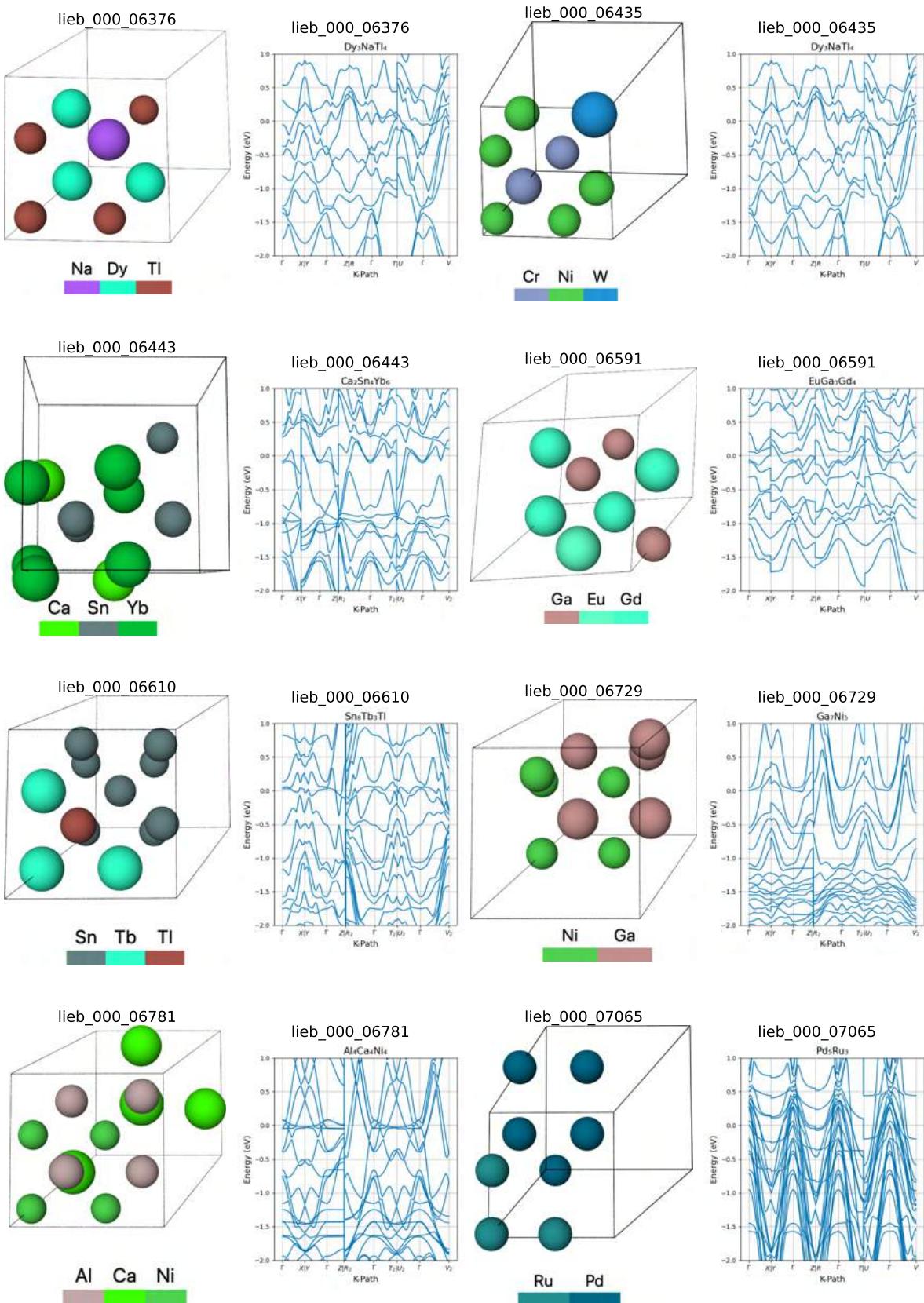


Figure S204. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

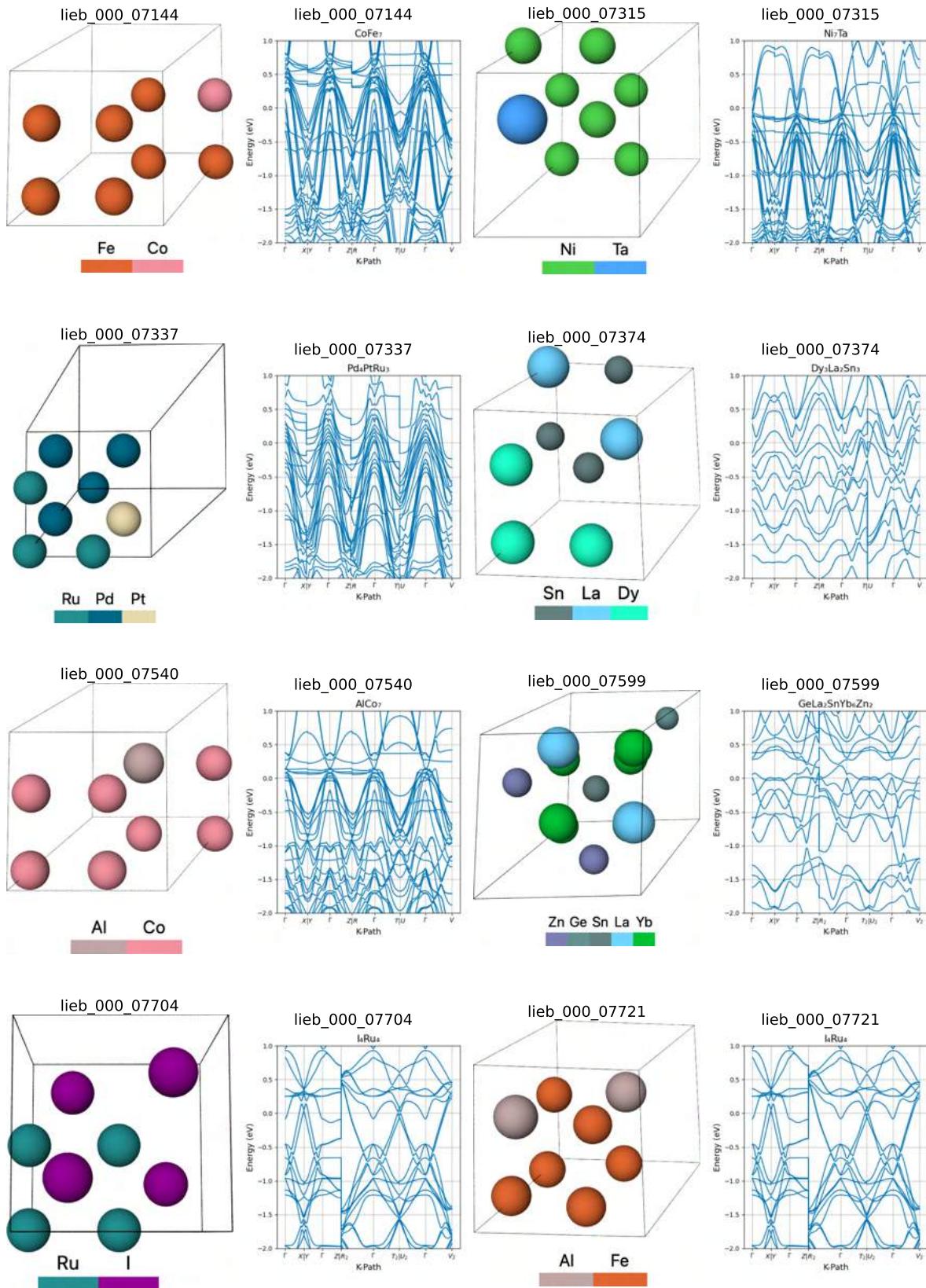


Figure S205. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

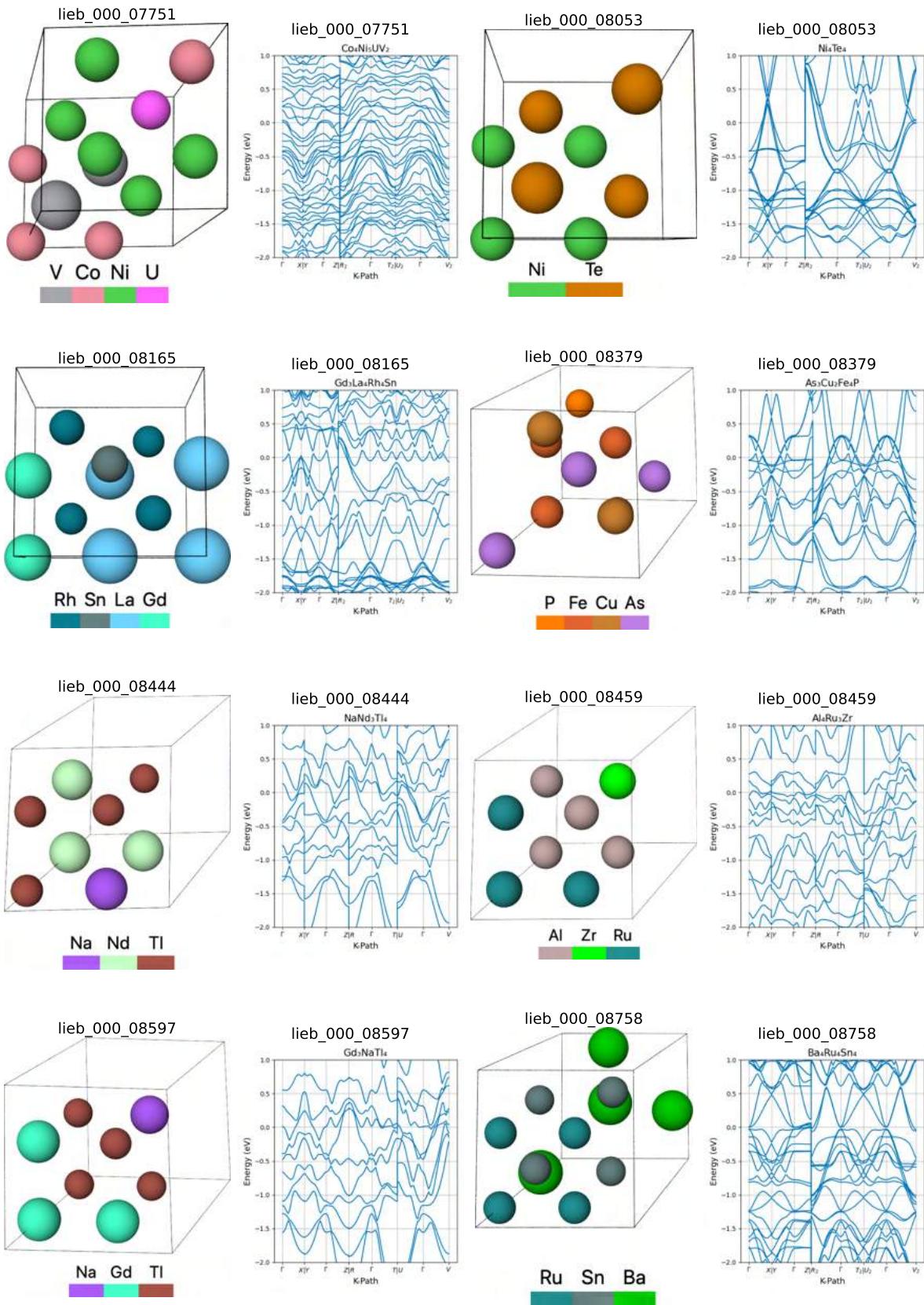


Figure S206. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

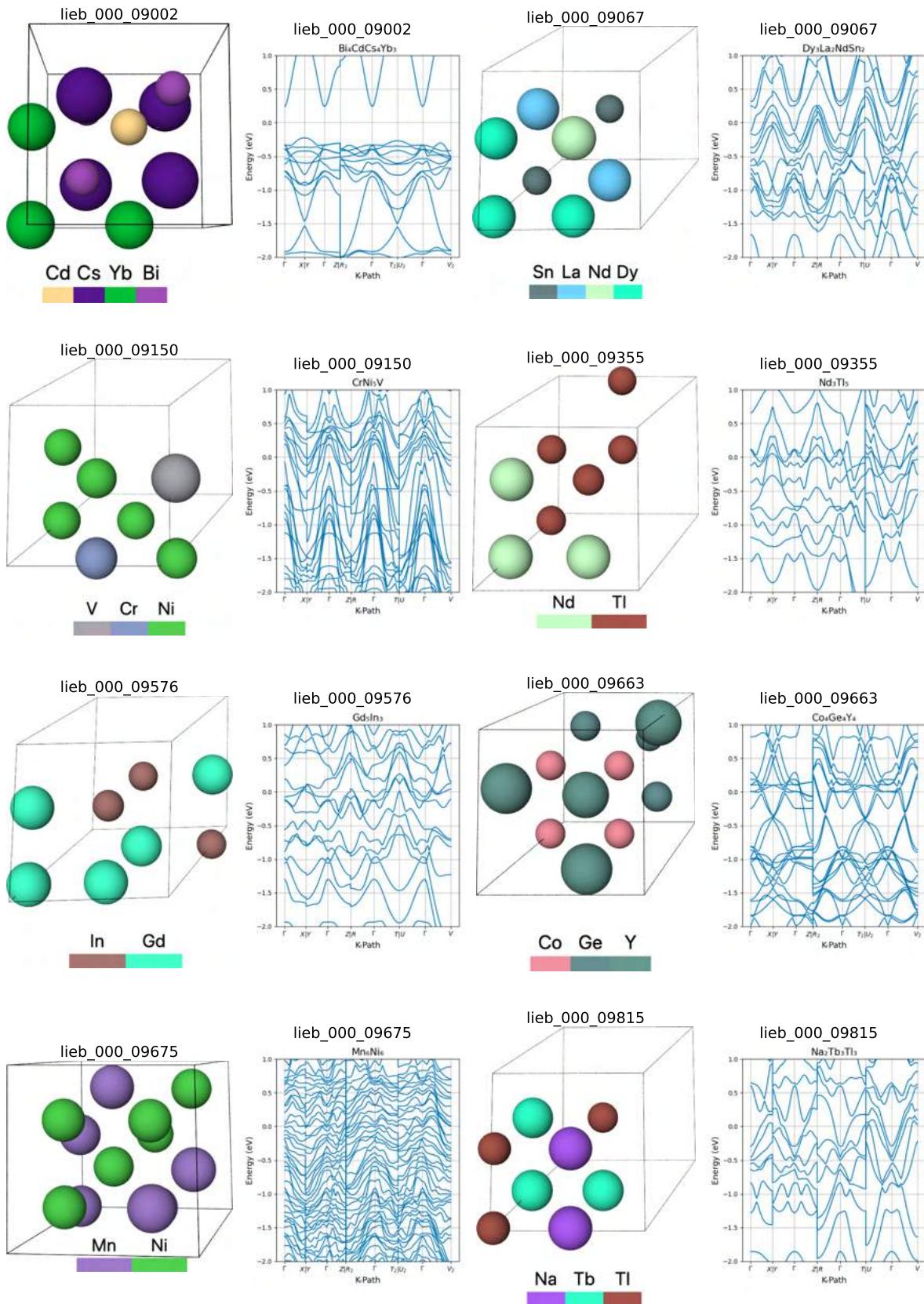


Figure S207. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

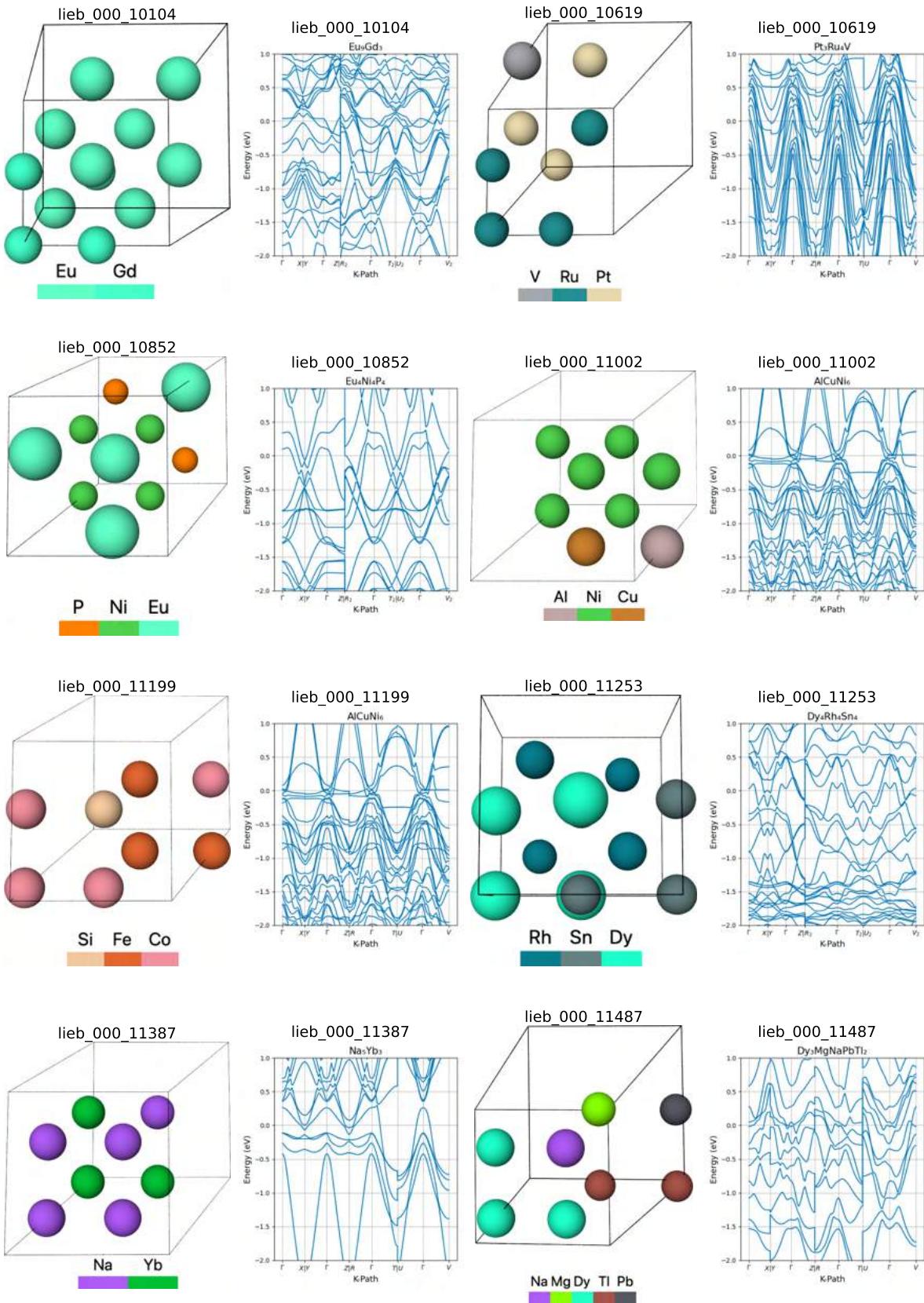


Figure S208. Generated materials with Lieb lattice structures and the corresponding band structures
We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

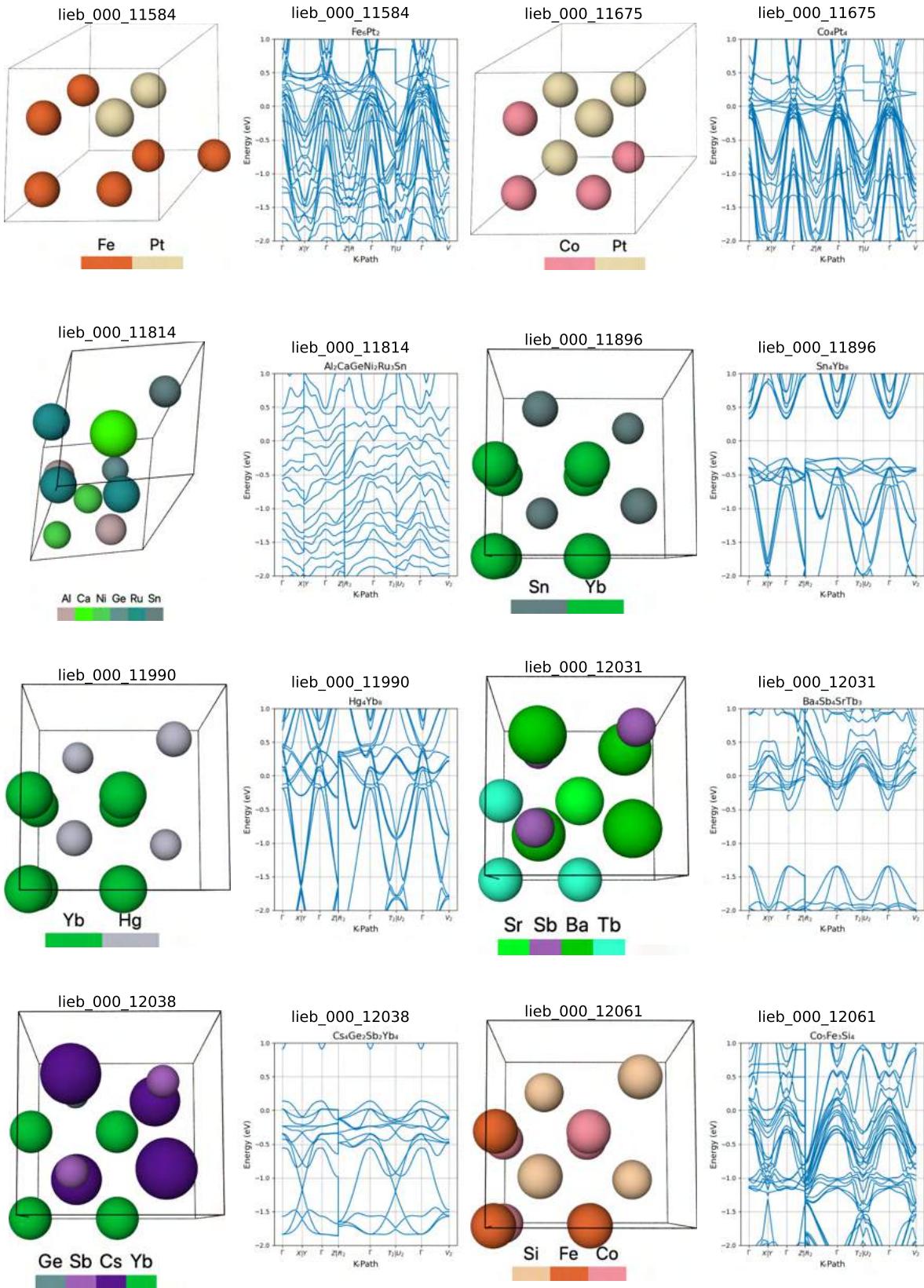


Figure S209. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

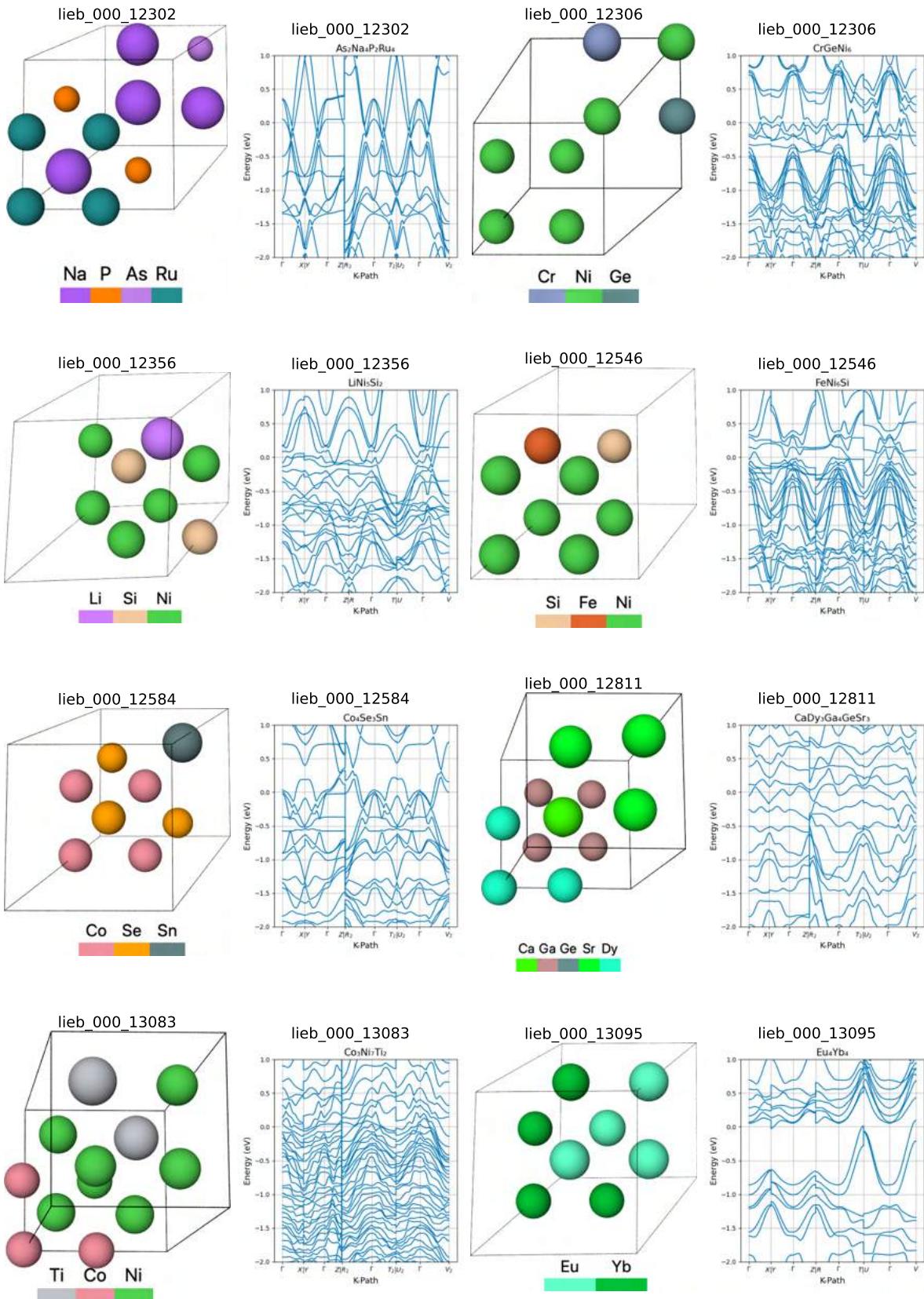


Figure S210. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

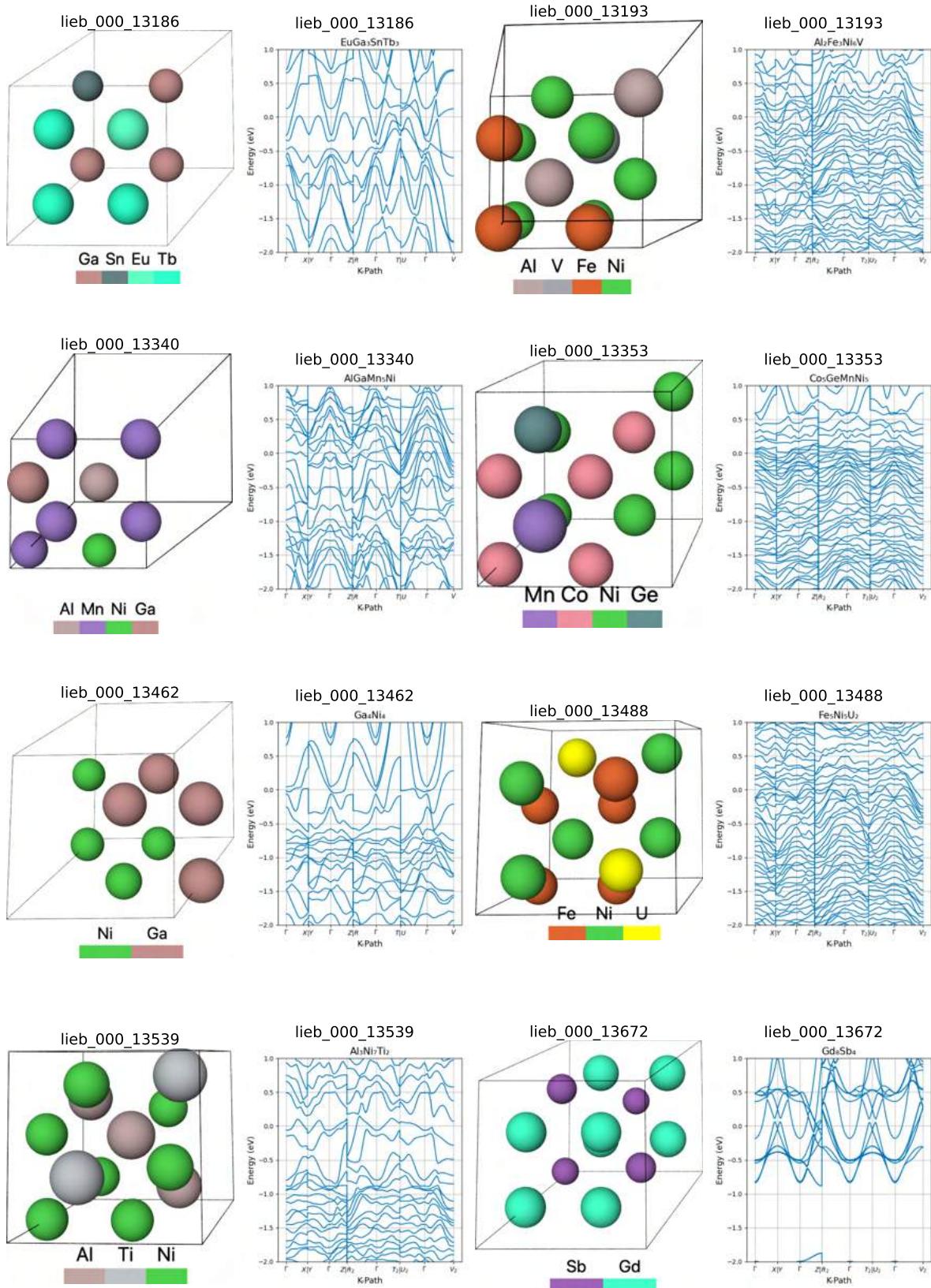


Figure S211. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

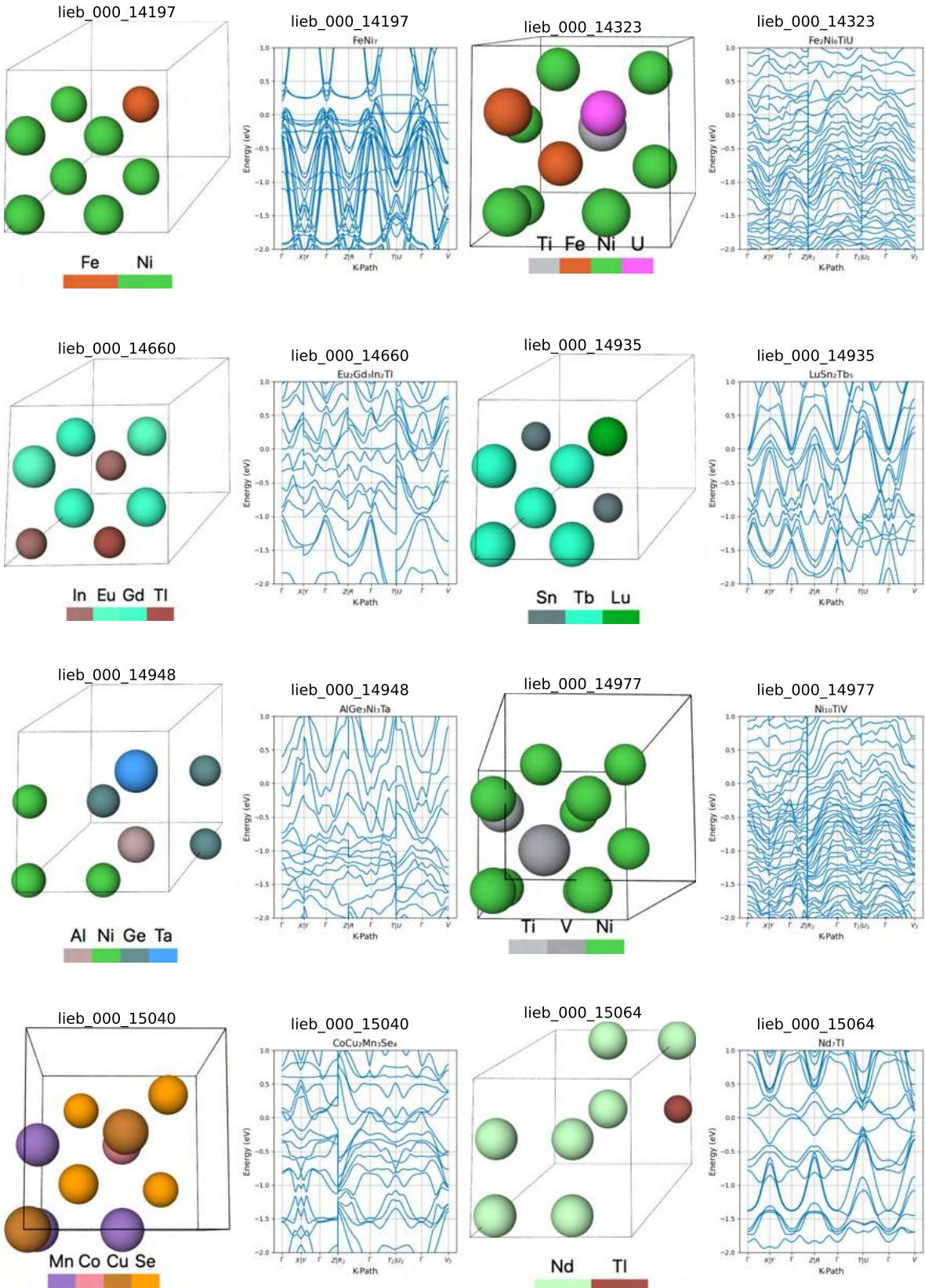


Figure S212. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

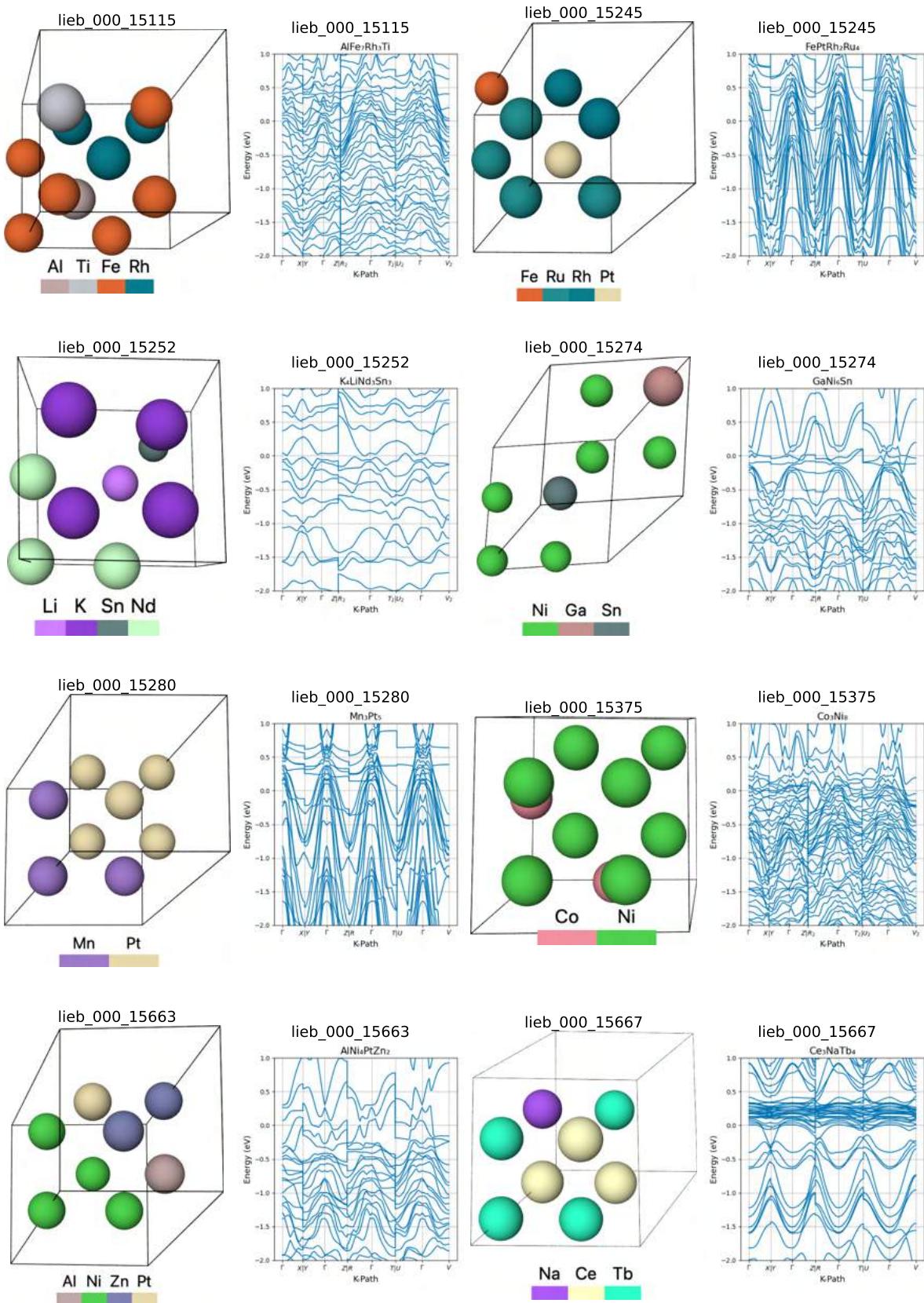


Figure S213. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

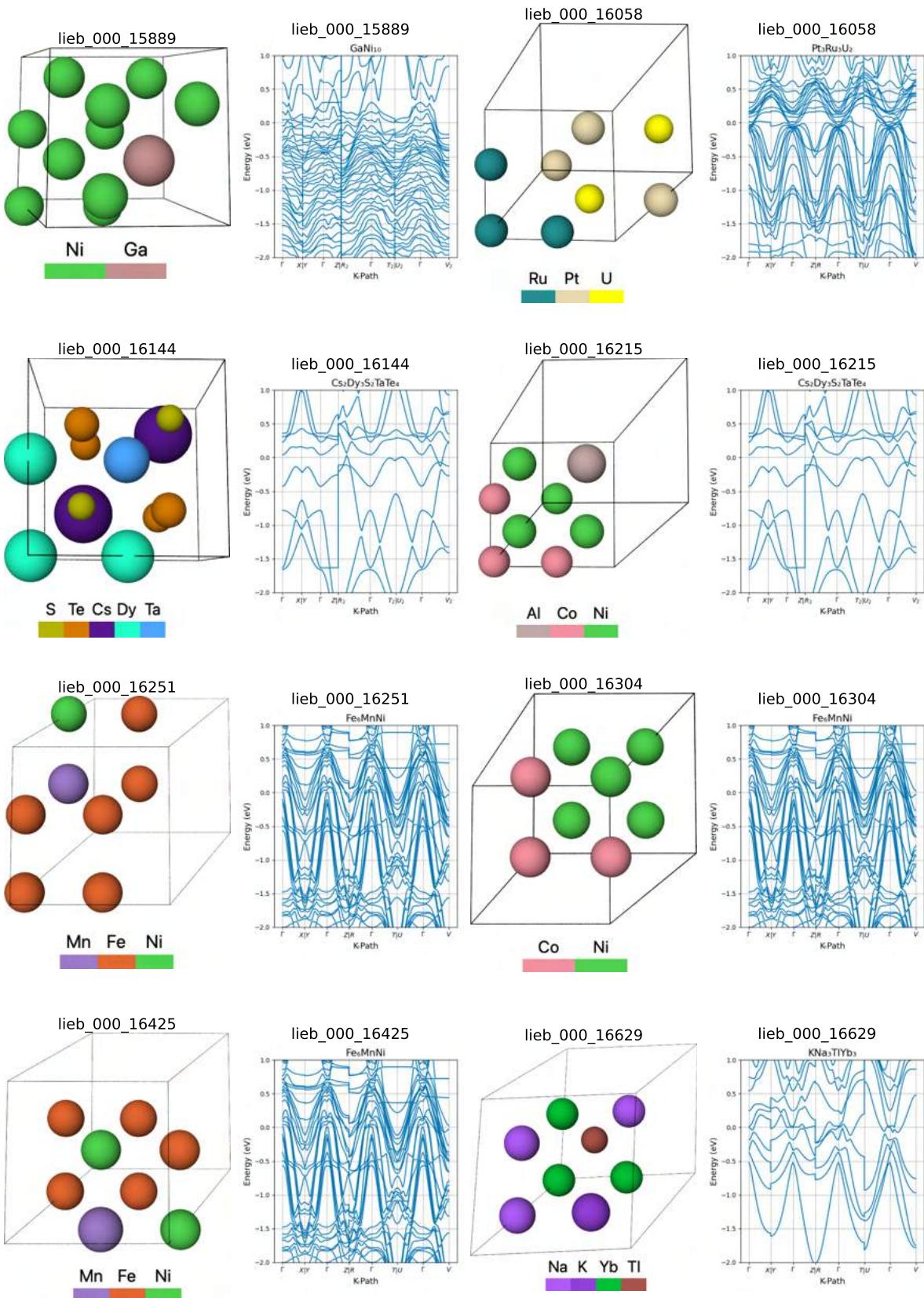


Figure S214. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

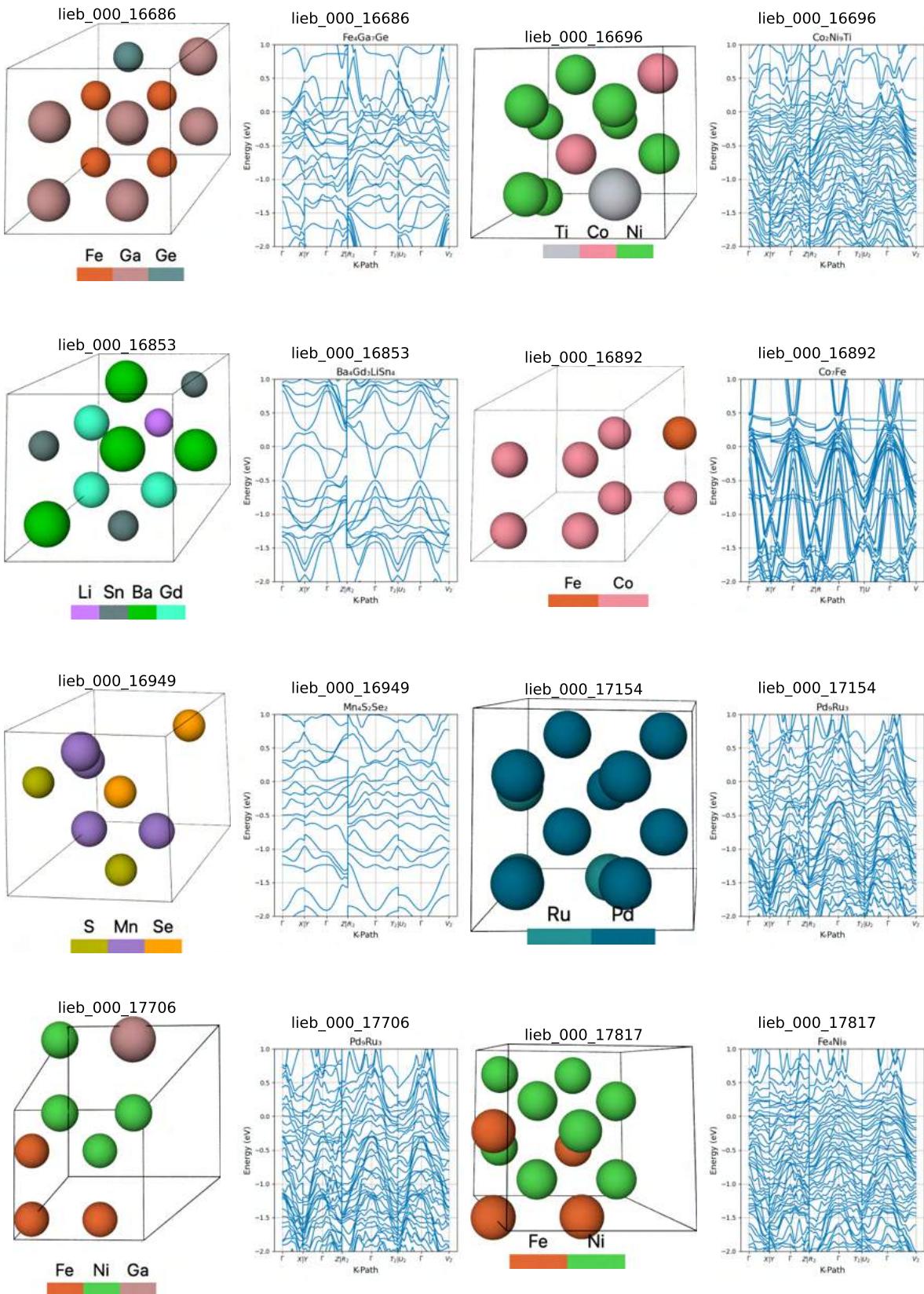


Figure S215. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

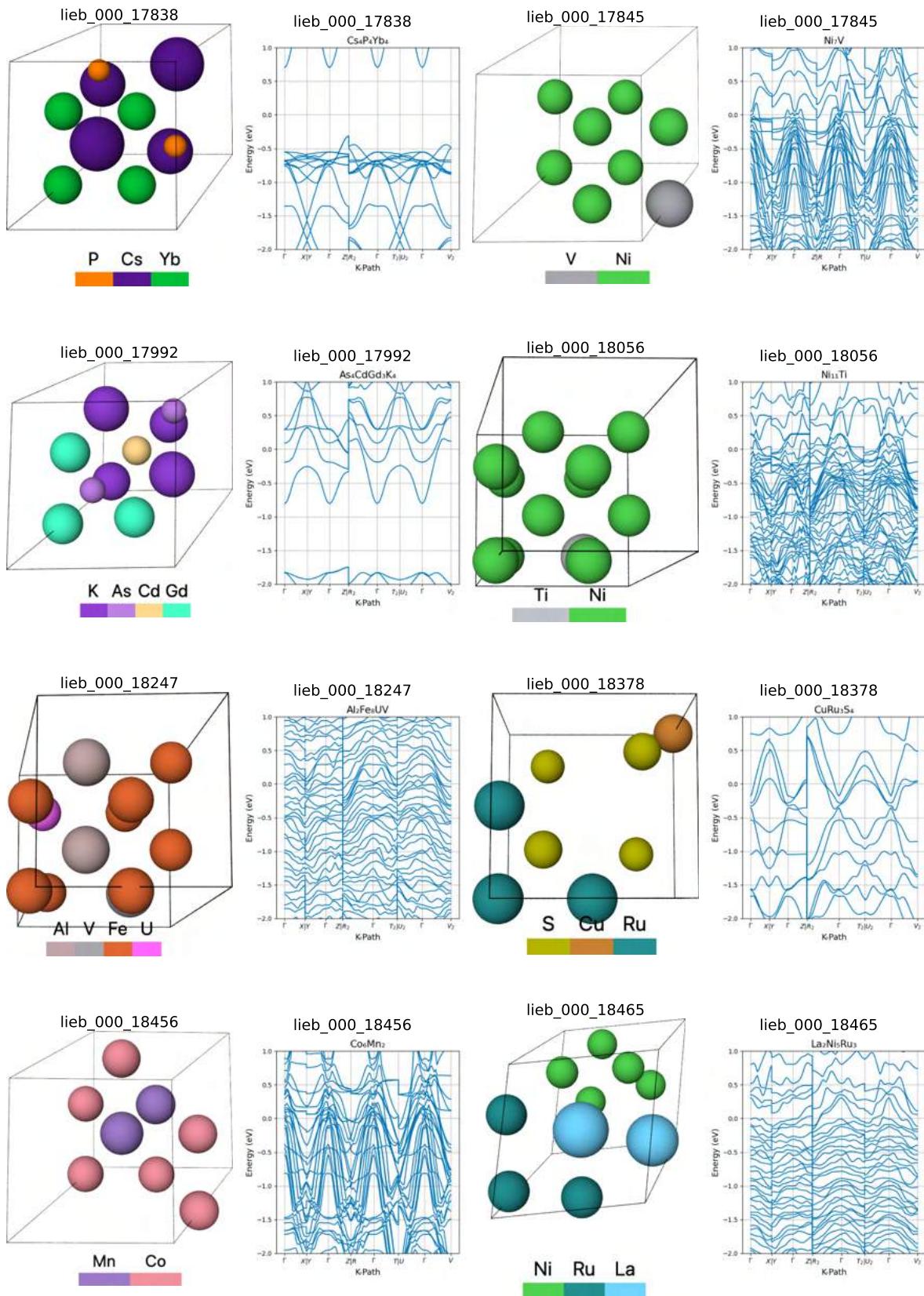


Figure S216. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

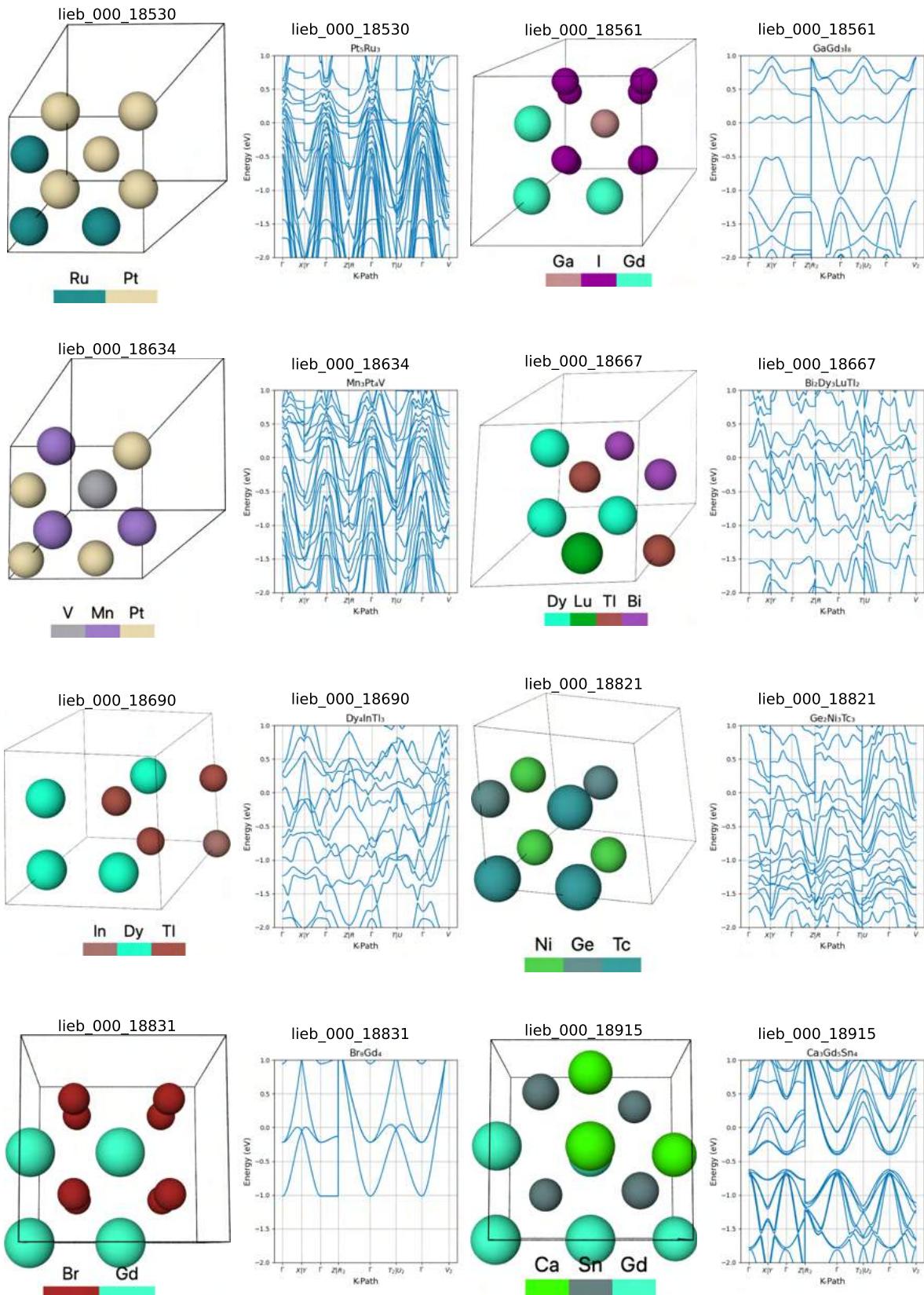


Figure S217. Generated materials with Lieb lattice structures and the corresponding band structures
 We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

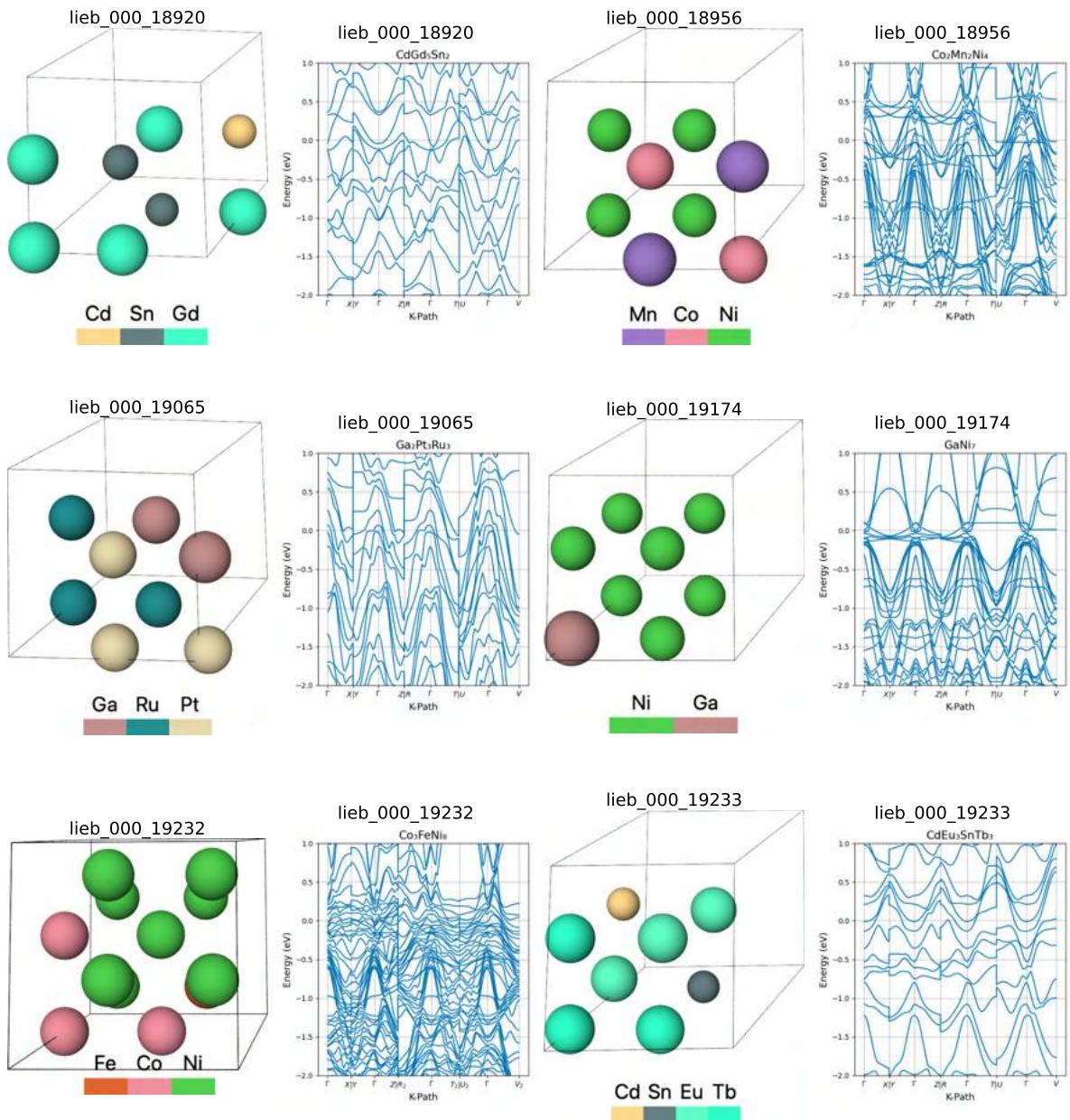


Figure S218. Generated materials with Lieb lattice structures and the corresponding band structures

We selected materials with $F_{max} = 0.01 \text{ eV}/\text{\AA}$, $d_{latt} = 1.0 \text{ \AA}$, and $d_{xy} = 0.5 \text{ \AA}$ as the thresholds.

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation

Index	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_00022	NdSiTe	3	-4.442	-4.911	-3.000e-06	0.00343	1.512	0.97
tri_000_00034	GdNiSi	3	-5.908	-5.929	-2.400e-05	0.00821	0.141	0.126
tri_000_00038	GeTbTe	3	-4.27	-4.731	-2.000e-06	0.0059	1.362	0.931
tri_000_00040	CoPb	2	-2.048	-4.604	-7.800e-06	0.00474	0.838	0.701
tri_000_00055	RuZr	2	-8.79	-8.964	4.000e-06	0.00283	0.338	0.154
tri_000_00076	CoTh	2	-5.176	-7.24	2.000e-06	0.00334	1.245	0.901
tri_000_00086	MnTi	2	-8.069	-8.454	-1.200e-05	0.00286	0.346	0.469
tri_000_00127	FeRh	2	-7.579	-7.616	-1.000e-06	0.00338	0.093	0.081
tri_000_00129	As ₂ HfYb	4	-5.954	-6.285	-1.000e-06	0.00526	0.41	0.85
tri_000_00163	GeNdSi	3	-5.373	-5.428	-1.000e-06	0.00534	0.207	0.124
tri_000_00170	GePdTb	3	-5.344	-5.724	0.000e+00	0.00372	0.668	0.812
tri_000_00184	MnZn	2	-4.429	-4.801	-5.000e-07	0.00143	0.355	0.071
tri_000_00188	Dy ₂	2	-4.524	-4.527	-9.000e-06	0.00416	0.038	0.022
tri_000_00191	TbYb	2	-2.824	-2.906	-6.400e-06	0.00276	0.319	0.392
tri_000_00226	NiRe	2	-8.407	-8.875	-9.100e-05	0.0068	0.284	0.233
tri_000_00250	NdSe	2	-5.296	-5.834	-3.000e-06	0.00125	0.501	0.286
tri_000_00253	H ₃ Nd	4	-4.206	-4.222	0.000e+00	0.00338	0.112	0.033
tri_000_00258	NdTe	2	-5.008	-5.299	-1.500e-05	0.0019	0.463	0.306
tri_000_00286	P ₂ Tb	3	-2.586	-5.919	-5.000e-06	0.0058	0.933	0.887
tri_000_00295	SnYb	2	-3.109	-3.153	-1.000e-06	0.00429	0.151	0.087
tri_000_00312	NdTm	2	-4.552	-4.556	4.500e-06	0.00048	0.057	0.042
tri_000_00326	B ₂ Ru	3	-7.207	-7.424	-6.000e-06	0.00565	0.267	0.219
tri_000_00327	IrNi	2	-7.045	-7.108	-2.000e-05	0.00164	0.139	0.144
tri_000_00351	TbYb	2	-2.905	-2.91	-1.240e-05	0.00133	0.082	0.067
tri_000_00376	Ir ₂ NdPr	4	-7.311	-7.382	-1.000e-06	0.00351	0.22	0.127
tri_000_00378	Dy ₂	2	-4.496	-4.522	-2.500e-06	0.0032	0.123	0.092
tri_000_00385	HfNd	2	-6.796	-7.036	-1.000e-06	0.00666	0.332	0.302
tri_000_00415	CuDySe ₂	4	-4.633	-4.998	0.000e+00	0.00936	0.463	0.793
tri_000_00431	AuMn	2	-5.169	-5.493	-1.000e-06	0.00127	0.509	0.377
tri_000_00524	DySTi	3	-6.087	-6.483	-4.000e-06	0.00542	0.234	0.372
tri_000_00530	MnTb	2	-5.313	-5.978	-2.200e-05	0.00299	0.74	0.766
tri_000_00541	ClCrDySe	4	-5.311	-5.484	-5.000e-06	0.00586	0.455	0.504
tri_000_00543	IrTeYb	3	-4.727	-5.151	-1.100e-05	0.00819	0.778	1.008
tri_000_00563	GaPdTb	3	-4.897	-5.073	0.000e+00	0.00431	0.467	0.403
tri_000_00565	GdY	2	-5.454	-5.504	-4.000e-06	0.00323	0.197	0.089
tri_000_00581	SSiTb	3	-4.797	-5.382	0.000e+00	0.00161	0.689	0.776
tri_000_00602	SeTb	2	-5.597	-5.704	1.000e-06	0.00061	0.202	0.164
tri_000_00605	AsBrSiYb	4	-3.785	-4.125	-1.000e-06	0.00615	0.649	0.685
tri_000_00610	CoSe ₂	3	-4.344	-4.954	0.000e+00	0.00735	0.586	0.46
tri_000_00616	B ₂ Ru	3	-7.147	-7.552	0.000e+00	0.00532	0.492	1.472
tri_000_00638	CDy	2	-5.699	-6.85	-1.000e-06	0.00238	0.681	2.461
tri_000_00656	GaYb	2	-2.346	-2.424	-2.700e-06	0.00104	0.27	0.328
tri_000_00724	FeIn	2	-3.987	-4.785	3.000e-07	0.00254	0.601	0.473
tri_000_00780	FeTe ₂	3	-1.447	-4.754	0.000e+00	0.00629	1.355	0.969
tri_000_00816	CdDyPd	3	-3.71	-4.065	0.000e+00	0.00662	0.957	0.707
tri_000_00818	H ₂ BeTb	4	-2.186	-3.919	1.000e-06	0.00637	0.664	0.755
tri_000_00876	MnV	2	-8.815	-9.128	0.000e+00	0.00489	0.32	0.282
tri_000_00898	DyY	2	-5.461	-5.483	0.000e+00	0.0024	0.112	0.082
tri_000_00902	CoGdS	3	-5.933	-6.34	-1.200e-05	0.00679	0.483	0.604
tri_000_00917	CuNi	2	-4.518	-4.572	-1.620e-05	0.00535	0.149	0.147
tri_000_00947	DyYb	2	-2.806	-2.882	-1.400e-06	0.00168	0.282	0.262
tri_000_00970	Al ₃ Dy	4	-3.875	-3.964	0.000e+00	0.00317	0.359	0.299

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_00980	H ₂ Yb	3	-2.143	-3.279	-1.300e-06	0.0008	0.361	0.815
tri_000_00993	AsDyNbP	4	-6.871	-7.149	-2.000e-06	0.00498	0.366	0.394
tri_000_01000	MnV	2	-8.95	-9.13	-1.000e-05	0.00296	0.183	0.119
tri_000_01064	CdTb	2	24.038	-1.546	-1.000e-07	0.00821	0.774	0.71
tri_000_01112	GdSn	2	-4.513	-4.865	-3.000e-07	0.00321	0.771	0.63
tri_000_01145	AlFePd	3	-5.586	-5.838	-1.000e-05	0.00886	0.246	0.165
tri_000_01175	CoDyTe	3	-4.949	-5.585	1.300e-05	0.00936	0.925	0.744
tri_000_01195	HoNi	2	-4.642	-5.156	-3.400e-05	0.00662	0.853	0.611
tri_000_01248	AuMnZr	3	-5.697	-6.709	1.000e-06	0.00877	0.523	0.424
tri_000_01278	S ₂ Tb	3	-5.441	-5.826	0.0000e+00	0.0042	1.58	1.651
tri_000_01279	IrNi	2	-7.038	-7.108	-1.900e-05	0.0059	0.143	0.133
tri_000_01285	CrDySe ₂	4	-5.953	-5.998	-1.000e-06	0.00462	0.365	1.089
tri_000_01291	RuSi ₂	3	-3.603	-6.498	-5.000e-06	0.00345	0.759	0.714
tri_000_01301	RuS ₂	3	-5.505	-6.022	-1.000e-06	0.00489	0.719	0.446
tri_000_01312	FeRe	2	-10.064	-10.243	-2.000e-06	0.00906	0.184	0.135
tri_000_01313	AuTb	2	-4.548	-4.667	-3.000e-06	0.00473	0.263	0.353
tri_000_01328	MnTe ₂ Yb	4	-4.326	-4.695	-1.000e-06	0.00444	0.404	0.363
tri_000_01340	DyTe ₂	3	-4.557	-4.653	-1.000e-06	0.00612	0.807	1.163
tri_000_01345	DyInPtTe	4	-4.575	-4.635	1.000e-06	0.00736	0.396	0.262
tri_000_01386	RuZr	2	-8.207	-9.005	-1.000e-06	0.00095	0.263	0.175
tri_000_01437	CaYb	2	-1.56	-1.681	3.600e-06	0.00108	0.765	0.855
tri_000_01438	CeYb	2	-3.249	-3.446	1.900e-06	0.00268	0.555	0.483
tri_000_01441	Ge ₂ NdNi	4	-5.212	-5.229	5.000e-06	0.00578	0.156	0.155
tri_000_01456	DyRu	2	-6.73	-6.793	-1.900e-05	0.00636	0.257	0.19
tri_000_01468	H ₂ Mn	3	-3.899	-4.93	-5.000e-06	0.0021	0.819	0.607
tri_000_01504	GdLaMgTb	4	-3.791	-3.814	0.0000e+00	0.00495	0.294	0.399
tri_000_01550	Se ₂ Tb	3	-4.493	-5.242	-1.000e-06	0.0036	0.934	0.715
tri_000_01559	SnYb	2	-2.84	-3.159	-2.800e-06	0.00478	0.455	0.557
tri_000_01564	GdTm	2	-4.451	-4.522	-1.700e-06	0.00043	0.233	0.195
tri_000_01567	Ru ₂	2	-8.91	-9.25	-2.200e-05	0.00603	0.293	0.21
tri_000_01576	HPtYb	3	-2.464	-4.399	-1.000e-06	0.00479	0.879	0.308
tri_000_01580	Nd ₂	2	-4.664	-4.685	9.500e-06	0.00207	0.174	0.22
tri_000_01586	HPTb	3	-4.844	-5.146	0.0000e+00	0.004	0.253	0.604
tri_000_01612	InYb	2	-2.274	-2.487	-2.660e-05	0.00429	0.811	0.76
tri_000_01619	BGdS	3	-4.69	-5.532	-1.000e-06	0.00489	1.497	1.988
tri_000_01625	CoFe	2	-7.38	-7.488	2.000e-06	0.00208	0.13	0.097
tri_000_01642	AuNd	2	-4.582	-4.676	-1.000e-07	0.00133	0.272	0.326
tri_000_01661	PTeYb	3	-3.5	-4.029	-5.000e-06	0.00443	1.998	1.283
tri_000_01682	HCoNi	3	-5.113	-5.184	-3.000e-06	0.00792	0.175	0.167
tri_000_01693	MgNTiYb	4	-4.473	-5.242	-1.000e-06	0.00386	0.907	1.003
tri_000_01737	CoPt	2	-6.117	-6.357	0.0000e+00	0.00509	0.252	0.212
tri_000_01749	GdNd	2	-4.583	-4.623	-2.660e-05	0.00113	0.249	0.253
tri_000_01787	MnPdTl	3	-7.08	-7.434	-3.500e-05	0.00422	0.431	0.404
tri_000_01791	Si ₂ Tb	3	-4.999	-5.671	0.0000e+00	0.00645	0.694	2.06
tri_000_01805	DyTb	2	-4.519	-4.535	-2.100e-06	0.00147	0.107	0.11
tri_000_01819	CBeRu	3	-6.914	-7.215	-7.000e-06	0.00722	0.473	0.743
tri_000_01822	Dy ₂	2	-4.501	-4.522	-4.300e-06	0.00388	0.106	0.117
tri_000_01823	RuZr	2	-8.917	-8.972	1.200e-05	0.00668	0.259	0.303
tri_000_01849	MnPSi	3	-5.629	-6.762	0.0000e+00	0.00234	0.97	0.52
tri_000_01852	MnZn	2	-4.678	-4.795	1.010e-05	0.00244	0.277	0.101
tri_000_01935	SiSnTb	3	-4.728	-4.947	-1.000e-06	0.00615	1.026	0.709
tri_000_01938	PtTbTe	3	-4.787	-5.57	-5.000e-06	0.00337	0.993	0.963

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_01960	HgYb	2	-1.144	-1.328	-1.600e-06	0.0009	0.405	0.363
tri_000_01961	CoOs	2	-8.118	-8.93	-5.000e-06	0.00805	0.532	0.333
tri_000_01995	NdTh	2	-5.993	-6.006	1.000e-06	0.00225	0.123	0.134
tri_000_01998	B ₂ Ru	3	-7.303	-7.612	2.000e-06	0.00707	0.815	0.109
tri_000_02002	B ₂ Ru	3	-7.2	-7.608	-1.000e-06	0.00492	0.916	0.978
tri_000_02009	MnOs	2	-9.968	-10.109	-1.000e-06	0.00423	0.159	0.19
tri_000_02028	TbTe	2	-4.728	-5.136	-1.000e-06	0.00503	0.584	0.622
tri_000_02084	GeSrTb	3	-2.923	-3.906	-1.200e-05	0.00862	0.647	0.4
tri_000_02103	CoPt	2	-5.933	-6.352	-4.000e-06	0.006	0.413	0.515
tri_000_02125	EuYb	2	-1.611	-1.641	1.100e-06	0.00135	0.243	0.31
tri_000_02129	GeNdSr	3	-3.692	-3.949	-2.000e-05	0.005	0.448	0.309
tri_000_02145	CoSi	2	-6.35	-6.603	4.000e-06	0.00043	0.29	0.202
tri_000_02150	FeOsV	3	-9.236	-9.456	-1.000e-06	0.00618	0.243	0.352
tri_000_02157	DySe ₂	3	-5.091	-5.243	-4.000e-06	0.00558	0.858	0.577
tri_000_02160	NiPd	2	-5.003	-5.195	1.000e-06	0.00331	0.273	0.205
tri_000_02174	Ni ₂	2	-5.365	-5.386	-8.000e-06	0.00976	0.127	0.111
tri_000_02190	Cl ₂ Gd	3	-4.352	-4.703	0.000e+00	0.00269	0.423	0.521
tri_000_02193	NaSrYb	3	-1.345	-1.402	-2.560e-05	0.00255	0.354	0.415
tri_000_02213	F ₃ Ru	4	-4.273	-4.829	-6.000e-06	0.00717	0.567	1.101
tri_000_02220	FeRu	2	-8.393	-8.61	-4.000e-06	0.0025	0.236	0.283
tri_000_02288	CoCrRh	3	-7.635	-7.844	-3.000e-06	0.00964	0.197	0.251
tri_000_02302	CoCrFe	3	-8.065	-8.093	-1.500e-05	0.00501	0.093	0.112
tri_000_02311	DyPr	2	-4.519	-4.595	5.900e-06	0.00083	0.286	0.264
tri_000_02319	FePd	2	-6.205	-6.329	1.000e-06	0.00255	0.259	0.352
tri_000_02336	GdSm	2	-4.597	-4.603	1.400e-06	0.00272	0.074	0.038
tri_000_02341	LiMn	2	-4.815	-5.071	-4.000e-06	0.00378	0.395	0.354
tri_000_02355	CoOs	2	-8.76	-8.987	-2.000e-06	0.00178	0.21	0.221
tri_000_02364	MnPt	2	-6.999	-7.449	-2.700e-05	0.00247	0.451	0.19
tri_000_02374	NdS	2	-6.223	-6.273	-1.000e-06	0.00326	0.147	0.146
tri_000_02395	CHDy	3	-2.595	-5.941	0.000e+00	0.00749	0.758	1.582
tri_000_02401	AlDyGeN	4	-4.755	-5.927	-3.000e-05	0.00887	1.024	1.695
tri_000_02402	GdPtTe	3	-5.468	-5.639	0.000e+00	0.00316	0.484	0.561
tri_000_02415	SnYb	2	-2.821	-3.144	-9.800e-06	0.00313	0.584	0.984
tri_000_02416	DyGeS	3	-4.66	-5.171	-4.000e-06	0.00829	0.608	1.017
tri_000_02424	HAIRu	3	-5.095	-5.657	-1.000e-06	0.00534	0.596	0.684
tri_000_02487	AlGaYb	3	-3.058	-3.129	-4.600e-06	0.00479	0.287	0.231
tri_000_02519	Se ₂ Tb	3	-5.067	-5.245	0.000e+00	0.00166	0.983	0.807
tri_000_02539	HBrTb	3	-3.888	-4.163	-1.000e-06	0.00499	0.925	0.891
tri_000_02542	NiSn ₂ Tb	4	-4.673	-4.801	-1.600e-05	0.00451	0.249	0.338
tri_000_02545	DyLu	2	-4.354	-4.489	-4.000e-07	0.00522	0.312	0.224
tri_000_02549	AuCuRu	3	-4.803	-5.107	-4.000e-06	0.00875	0.427	0.414
tri_000_02554	MgNd	2	-3.003	-3.054	-9.000e-07	0.00184	0.264	0.3
tri_000_02586	EuYb	2	-1.622	-1.642	-6.000e-07	0.00208	0.236	0.167
tri_000_02595	NiOs	2	-7.776	-8.191	-1.000e-06	0.00452	0.348	0.277
tri_000_02628	GdRu	2	-6.243	-6.756	-1.700e-05	0.00234	0.342	0.164
tri_000_02636	CBeMn	3	-6.967	-7.315	-7.000e-06	0.0079	0.537	0.562
tri_000_02646	EuTb	2	-3.077	-3.091	-2.700e-06	0.00367	0.125	0.099
tri_000_02672	Br ₂ Tb	3	-3.981	-4.241	2.000e-06	0.00687	0.436	0.348
tri_000_02713	H ₂ Fe	3	-3.968	-4.817	-2.000e-06	0.00305	0.771	0.786
tri_000_02714	FePt	2	-6.475	-6.962	-6.000e-06	0.00786	0.497	0.299
tri_000_02765	TeYb	2	-3.512	-3.816	-1.560e-05	0.00182	0.473	0.429
tri_000_02811	GeNdPdSb	4	-4.758	-5.217	-1.000e-06	0.00362	0.417	0.344

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_02831	DySe	2	-5.481	-5.673	1.000e-06	0.0023	0.291	0.148
tri_000_02847	DyNZn	3	-5.15	-5.388	-3.000e-06	0.00359	0.521	0.953
tri_000_02858	CBeCo	3	-6.115	-6.349	0.000e+00	0.00545	0.556	0.578
tri_000_02908	BrNdPt	3	-4.348	-5.216	0.000e+00	0.00501	0.382	0.835
tri_000_02917	CDy ₂	3	-6.244	-6.364	0.000e+00	0.0097	0.245	0.191
tri_000_02932	NiOs	2	-7.954	-8.192	-6.000e-06	0.00551	0.127	0.036
tri_000_02943	PtTeYb	3	-4.022	-4.626	0.000e+00	0.0056	1.023	2.71
tri_000_02949	BaGdP	3	-4.17	-4.641	0.000e+00	0.00413	0.367	0.251
tri_000_02963	CrGdS	3	-6.081	-6.529	0.000e+00	0.00412	0.321	0.466
tri_000_02983	BRuY	3	-6.048	-7.86	-3.000e-06	0.00284	0.467	0.207
tri_000_02984	GdNd	2	-4.618	-4.629	-2.430e-05	0.00085	0.126	0.138
tri_000_03017	NdTb	2	-4.586	-4.613	3.600e-06	0.00203	0.13	0.053
tri_000_03018	CoRh	2	-6.802	-6.962	-1.700e-05	0.00693	0.214	0.199
tri_000_03021	Si ₂ Yb	3	-4.364	-4.463	-6.000e-06	0.00659	0.207	0.253
tri_000_03022	CoMn	2	-7.854	-7.98	-5.000e-06	0.00984	0.134	0.116
tri_000_03074	NdTh	2	5.078	-5.675	0.000e+00	0.00789	0.923	0.827
tri_000_03087	GaNdSi	3	-4.981	-5.038	-2.000e-06	0.00792	0.162	0.143
tri_000_03113	HgTb	2	26.719	-2.574	-2.200e-06	0.00439	0.962	1.558
tri_000_03117	GdTb	2	-4.553	-4.562	-1.400e-06	0.00063	0.092	0.081
tri_000_03146	HfNd	2	-6.832	-7.035	1.000e-06	0.00413	0.265	0.122
tri_000_03170	H ₂ Co	3	-3.05	-4.486	0.000e+00	0.00716	0.382	0.528
tri_000_03176	SnTb	2	-4.462	-4.697	-8.400e-06	0.00319	0.584	0.226
tri_000_03192	GdPtTe	3	-5.376	-5.638	-1.000e-06	0.00395	0.846	0.883
tri_000_03197	Dy ₂	2	-4.517	-4.526	2.000e-06	0.00365	0.089	0.082
tri_000_03198	EuGd	2	-3.061	-3.118	-4.100e-06	0.00262	0.254	0.176
tri_000_03202	Nd ₂	2	-4.622	-4.681	-5.400e-06	0.00673	0.363	0.336
tri_000_03222	DyY	2	-5.461	-5.477	-8.000e-06	0.00037	0.127	0.072
tri_000_03253	Nd ₂ Si	3	-3.843	-5.364	0.000e+00	0.00307	1.311	1.131
tri_000_03254	CBFe	3	-7.485	-7.853	0.000e+00	0.00857	0.474	0.491
tri_000_03286	MgNNd	3	-5.383	-5.457	-2.300e-05	0.00467	0.195	0.241
tri_000_03289	S ₂ Tb	3	-5.339	-5.737	0.000e+00	0.00307	0.713	0.871
tri_000_03300	Ga ₂ Yb	3	-2.923	-2.98	-1.000e-07	0.00697	0.335	0.316
tri_000_03310	BrSiYb	3	-0.689	-3.18	-2.900e-06	0.00394	0.995	0.853
tri_000_03357	CrPtTbTe	4	-5.576	-6.082	9.000e-06	0.00619	0.562	0.523
tri_000_03398	GdS ₂	3	-5.291	-5.84	-2.000e-06	0.00476	1.6	1.633
tri_000_03399	EuNd	2	-3.161	-3.21	-1.200e-06	0.00044	0.296	0.381
tri_000_03404	STbZn	3	-3.785	-4.151	-3.000e-06	0.00641	0.553	0.742
tri_000_03424	Fe ₂	2	-7.991	-8.154	-3.000e-06	0.00265	0.188	0.206
tri_000_03438	CGdSb	3	-5.557	-5.884	0.000e+00	0.00395	0.543	0.509
tri_000_03441	DyYb	2	-2.827	-2.886	1.600e-06	0.00368	0.291	0.212
tri_000_03464	PdRu	2	-6.933	-6.982	-1.100e-05	0.00253	0.109	0.118
tri_000_03486	DySe ₂	3	-4.856	-5.233	-1.000e-06	0.00475	0.808	0.683
tri_000_03542	PTeYb	3	-3.363	-3.964	-7.000e-06	0.00452	1.46	1.091
tri_000_03545	MnV	2	-8.935	-9.129	0.000e+00	0.00516	0.21	0.089
tri_000_03548	CaITb	3	-5.855	-6.068	0.000e+00	0.00833	0.319	0.312
tri_000_03554	TbTh	2	-5.941	-5.95	5.000e-06	0.00178	0.102	0.144
tri_000_03559	CaITb	3	-5.971	-6.068	0.000e+00	0.00486	0.16	0.155
tri_000_03590	FePd	2	-6.213	-6.327	1.000e-06	0.00283	0.228	0.243
tri_000_03592	AcDy	2	-4.195	-4.205	-3.200e-06	0.00419	0.099	0.052
tri_000_03598	PdYb	2	-3.895	-4.201	-2.000e-07	0.00224	0.848	0.596
tri_000_03605	DyGaP	3	-4.488	-4.984	0.000e+00	0.00458	1.089	0.542
tri_000_03612	AsDyPt ₂	4	-5.318	-6.093	-1.500e-05	0.00805	0.794	0.755

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_03614	H ₂ Mn	3	-3.036	-5.067	-9.000e-06	0.00311	0.366	0.404
tri_000_03623	PdRu	2	-6.675	-6.994	-1.000e-06	0.00095	0.537	0.392
tri_000_03633	CaNd	2	-3.226	-3.244	7.000e-07	0.0007	0.152	0.151
tri_000_03709	Tb ₂	2	-4.545	-4.552	-2.400e-06	0.00216	0.079	0.078
tri_000_03731	GdPdSb ₂	4	-5.157	-5.197	2.000e-06	0.00239	0.137	0.175
tri_000_03796	AlGaNd	3	-4.35	-4.385	0.000e+00	0.00357	0.139	0.09
tri_000_03809	CaNd	2	-3.179	-3.243	-8.000e-07	0.00149	0.261	0.167
tri_000_03810	CeYb	2	-3.281	-3.446	-2.450e-05	0.00347	0.54	0.329
tri_000_03849	NdSbSi	3	-4.783	-5.201	-2.000e-06	0.00429	0.738	0.646
tri_000_03851	AuMn	2	-5.319	-5.484	0.000e+00	0.0046	0.318	0.229
tri_000_03867	HoRu	2	-6.442	-6.816	-7.000e-06	0.00651	0.533	0.295
tri_000_03871	NiSc	2	-5.798	-6.06	-8.900e-05	0.00452	0.757	0.794
tri_000_03889	AlCo	2	-5.273	-5.706	-4.300e-05	0.00694	0.463	0.616
tri_000_03894	DyGeP	3	-3.679	-5.409	-1.500e-05	0.00829	0.99	0.736
tri_000_03992	NiZn	2	-3.33	-3.433	-4.200e-06	0.00169	0.24	0.266
tri_000_04027	HfSb ₂ Yb	4	-5.522	-5.632	0.000e+00	0.00339	0.225	1.319
tri_000_04098	AuRu	2	-5.334	-5.737	-1.000e-06	0.00173	0.387	0.354
tri_000_04106	DyNi	2	-3.243	-4.968	-7.060e-05	0.00693	0.873	0.589
tri_000_04123	CoGa	2	-4.905	-5.091	-1.600e-05	0.00501	0.279	0.295
tri_000_04135	FeTe ₂	3	-4.475	-4.87	1.000e-06	0.00619	0.346	0.211
tri_000_04150	GdSn	2	-4.691	-4.702	-1.930e-05	0.00622	0.091	0.13
tri_000_04156	Dy ₂	2	-4.462	-4.522	-3.000e-07	0.0024	0.23	0.338
tri_000_04202	AcGd	2	-4.156	-4.248	5.700e-06	0.00441	0.234	0.194
tri_000_04204	CDyGe	3	-6.014	-6.065	4.000e-06	0.00591	0.42	0.244
tri_000_04228	NiSiYb	3	-4.664	-4.678	2.000e-06	0.00183	0.068	0.038
tri_000_04230	MnPd	2	-6.589	-6.811	-2.000e-06	0.00497	0.287	0.286
tri_000_04241	MnPt	2	-7.095	-7.451	0.000e+00	0.00515	0.43	0.302
tri_000_04247	NdTe ₂	3	-4.466	-4.722	0.000e+00	0.00959	1.334	0.993
tri_000_04297	NiTa	2	-8.361	-8.774	-2.400e-05	0.00144	0.474	0.258
tri_000_04342	PtTbTe	3	-5.442	-5.614	0.000e+00	0.00686	0.694	0.788
tri_000_04350	GdSi ₂	3	-5.652	-5.701	0.000e+00	0.00391	0.287	0.106
tri_000_04383	GdZr	2	-6.341	-6.421	-8.000e-06	0.00273	0.257	0.139
tri_000_04402	C ₃ Gd	4	-6.057	-7.768	-1.000e-06	0.00851	0.624	0.699
tri_000_04419	FeO ₂	3	-7.001	-7.018	-9.000e-06	0.00867	0.117	0.147
tri_000_04425	NdNiSi	3	-5.882	-5.911	-2.000e-05	0.00951	0.1	0.06
tri_000_04444	CsYb	2	-0.495	-0.883	-1.000e-07	0.00124	0.925	0.667
tri_000_04482	NaYb	2	-1.24	-1.309	-2.500e-06	0.00079	0.37	0.678
tri_000_04487	DySSe	3	-5.288	-5.529	-2.000e-06	0.00459	1.423	1.011
tri_000_04507	DyFeSi	3	-6.338	-6.502	0.000e+00	0.00304	0.263	0.255
tri_000_04517	SnYb	2	-2.743	-3.159	-4.600e-06	0.00561	0.536	0.536
tri_000_04534	CoGa	2	-4.985	-5.092	-4.000e-06	0.005	0.218	0.152
tri_000_04537	DyPtSb	3	-5.738	-5.958	5.000e-06	0.00499	0.232	0.297
tri_000_04558	B ₂ Ru	3	-7.37	-7.561	0.000e+00	0.00548	0.952	0.972
tri_000_04562	DyPb	2	-4.362	-4.374	2.900e-06	0.00387	0.111	0.141
tri_000_04565	CdMgMn	3	-2.703	-3.207	-1.000e-07	0.00387	0.607	0.614
tri_000_04586	DyTaTe	3	-6.505	-6.624	0.000e+00	0.00194	0.319	0.308
tri_000_04588	ScTb	2	-5.349	-5.362	-1.000e-06	0.00358	0.099	0.079
tri_000_04611	DyTm	2	-4.448	-4.496	-1.080e-05	0.00352	0.164	0.132
tri_000_04612	Se ₂ Tb	3	-4.712	-5.237	0.000e+00	0.00538	0.926	1.02
tri_000_04631	PdSeTb	3	-5.254	-5.551	0.000e+00	0.00754	0.781	0.995
tri_000_04659	TbTeV	3	-5.265	-5.642	1.000e-06	0.00899	0.446	0.358
tri_000_04682	RuZn	2	-4.995	-5.067	-1.000e-06	0.00264	0.176	0.172

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_04695	AlAuCo	3	-4.539	-4.697	-8.000e-05	0.00702	0.142	0.206
tri_000_04707	DyS ₂	3	-5.312	-5.799	-1.000e-06	0.00629	1.782	1.16
tri_000_04713	NdTm	2	-4.541	-4.555	1.810e-05	0.00173	0.121	0.103
tri_000_04717	MnTi	2	-8.238	-8.453	1.000e-06	0.00057	0.213	0.165
tri_000_04729	NdRh ₂ Se	4	-5.744	-6.21	2.000e-06	0.00526	0.745	0.919
tri_000_04730	CoTc	2	-8.374	-8.604	-5.000e-06	0.00378	0.17	0.133
tri_000_04847	B ₂ Ru	3	-7.319	-7.393	-2.000e-06	0.00166	0.166	0.094
tri_000_04866	Cl ₂ Co	3	-2.156	-3.863	-1.000e-06	0.00977	0.527	0.335
tri_000_04871	NdRu	2	-6.31	-6.684	-2.000e-06	0.00349	0.438	0.486
tri_000_04900	TbYb	2	-0.965	-2.769	-5.700e-06	0.00351	0.805	0.504
tri_000_04906	AuRu	2	-4.975	-5.683	-2.000e-06	0.00572	0.456	0.299
tri_000_04915	MnTc	2	-9.25	-9.496	-7.400e-05	0.00342	0.427	0.34
tri_000_04918	DyY	2	-5.432	-5.483	-9.000e-06	0.00246	0.228	0.172
tri_000_04929	AgNi ₂	3	-4.041	-4.297	-1.000e-06	0.00444	0.284	0.389
tri_000_04951	RuZr	2	-8.668	-8.939	0.000e+00	0.00635	0.366	0.329
tri_000_04959	SmTb	2	-4.577	-4.589	-7.600e-06	0.00148	0.087	0.071
tri_000_04987	CeTb	2	-5.022	-5.132	4.000e-06	0.00855	0.371	0.218
tri_000_04994	HCoSiTb	4	-5.621	-5.682	0.000e+00	0.00558	0.228	0.157
tri_000_05014	NdRu	2	-6.349	-6.899	1.000e-06	0.00538	0.875	0.876
tri_000_05055	GdMn ₂ Si	4	3.713	-6.824	1.000e-06	0.00668	1.028	2.035
tri_000_05082	NdSn	2	-4.693	-4.75	5.000e-07	0.00924	0.224	0.233
tri_000_05097	NdPtS	3	-5.527	-6.157	7.000e-06	0.00958	0.937	0.859
tri_000_05099	AsFe	2	-5.551	-6.31	1.000e-06	0.00748	0.562	0.484
tri_000_05139	DyGeS	3	-4.808	-5.176	-2.000e-06	0.00682	0.623	0.733
tri_000_05140	CoMnSSi	4	-6.444	-6.605	1.000e-06	0.00389	0.303	0.256
tri_000_05148	CoCr	2	-8.137	-8.167	-5.000e-06	0.00438	0.102	0.083
tri_000_05151	GdLu	2	-4.379	-4.506	-5.900e-06	0.00386	0.274	0.126
tri_000_05165	HRuSe	3	-4.935	-5.149	0.000e+00	0.00246	0.572	0.634
tri_000_05176	GaGeYb	3	-3.247	-3.532	-1.500e-05	0.00906	0.516	0.373
tri_000_05188	NdTh	2	-5.974	-6.006	-2.000e-06	0.00523	0.188	0.092
tri_000_05219	NdYb	2	-2.982	-3.027	1.050e-05	0.0043	0.265	0.2
tri_000_05257	NdYb	2	-2.98	-3.03	-2.500e-06	0.00184	0.27	0.179
tri_000_05290	CrCuNiRu	4	-6.434	-6.814	7.000e-06	0.00522	0.599	0.683
tri_000_05294	Ni ₂	2	-5.336	-5.384	-5.000e-06	0.0043	0.181	0.234
tri_000_05295	AgAs ₂ Yb	4	-3.601	-3.672	0.000e+00	0.00353	0.232	0.23
tri_000_05303	Cl ₂ Ru	3	-4.393	-4.568	-2.000e-06	0.00571	0.301	2.295
tri_000_05313	DyY	2	-5.438	-5.485	-3.000e-06	0.00081	0.189	0.156
tri_000_05316	AsNi	2	-4.485	-5.103	-7.000e-06	0.00287	0.467	0.506
tri_000_05320	DyLu	2	-4.471	-4.486	-1.000e-06	0.00255	0.13	0.085
tri_000_05345	NdO	2	-7.123	-7.326	-1.000e-06	0.00378	0.226	0.204
tri_000_05355	FeSeTb	3	-5.533	-6.074	3.000e-06	0.00945	0.87	2.379
tri_000_05374	DySe ₂	3	-4.51	-5.222	0.000e+00	0.00446	0.755	0.907
tri_000_05376	GaSbTb	3	-4.042	-4.335	-1.000e-06	0.00446	0.49	0.271
tri_000_05395	CoNi	2	-6.004	-6.055	-6.800e-05	0.00914	0.144	0.085
tri_000_05400	B ₂ Ru	3	-7.155	-7.4	-1.000e-05	0.00604	0.198	0.152
tri_000_05401	B ₂ Ru	3	-7.008	-7.547	0.000e+00	0.00384	0.517	0.906
tri_000_05411	GdSi ₂	3	-0.864	-5.645	1.000e-05	0.00415	0.976	1.087
tri_000_05431	GdRuSe	3	-5.933	-6.497	-1.000e-06	0.00471	1.008	2.327
tri_000_05451	Te ₂ VYb	4	-4.379	-4.812	4.000e-06	0.00894	0.453	1.297
tri_000_05462	LiMg ₂ Nd	4	-1.759	-2.468	-9.000e-07	0.00374	0.836	0.452
tri_000_05490	BaDy	2	-2.742	-2.904	-2.030e-05	0.00444	0.349	0.206
tri_000_05508	CoGa	2	-4.803	-5.087	0.000e+00	0.00283	0.276	0.193

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_05535	CoZn	2	-3.979	-3.984	-3.000e-07	0.00219	0.036	0.061
tri_000_05547	CDyTi	3	-7.226	-7.546	-1.000e-06	0.00982	0.534	0.63
tri_000_05548	PSeYb	3	-3.569	-4.272	-6.000e-06	0.00685	1.068	0.995
tri_000_05561	FeOs	2	-9.423	-9.649	-4.000e-06	0.00288	0.19	0.151
tri_000_05565	AcDy	2	-4.085	-4.204	-4.300e-06	0.00185	0.277	0.16
tri_000_05594	GdPr	2	-4.609	-4.634	-2.900e-06	0.00344	0.181	0.204
tri_000_05598	NdSn	2	-4.675	-4.957	1.500e-06	0.00249	0.8	0.626
tri_000_05599	CuPdTb	3	-4.447	-5.083	-2.000e-06	0.00374	0.519	0.644
tri_000_05605	NdSbT ₂	4	-5.411	-5.992	0.000e+00	0.00545	1.223	2.569
tri_000_05616	AuNi	2	-3.539	-4.129	-2.130e-05	0.00932	0.265	0.142
tri_000_05620	BiCuDy	3	-4.312	-4.472	-1.000e-05	0.00338	0.354	0.5
tri_000_05651	NiTm	2	-4.72	-5.348	-3.000e-06	0.00655	1.136	0.762
tri_000_05672	FeIr	2	-8.324	-8.517	-9.000e-06	0.00268	0.216	0.142
tri_000_05680	NiOs	2	-7.534	-8.19	-5.200e-05	0.00464	0.303	0.285
tri_000_05696	TbTm	2	-4.499	-4.51	-4.000e-07	0.00177	0.082	0.051
tri_000_05704	InTb	2	-3.814	-3.838	1.000e-05	0.00275	0.106	0.109
tri_000_05726	AuNdSn ₂	4	-4.306	-4.33	-1.000e-06	0.00294	0.103	0.12
tri_000_05737	AuMn	2	-5.187	-5.474	-7.000e-06	0.00398	0.513	0.443
tri_000_05748	BiMn	2	-2.884	-5.408	-1.000e-06	0.00249	0.852	1.018
tri_000_05767	CdNaTb	3	-1.908	-2.179	-7.000e-06	0.00548	1.314	2.81
tri_000_05773	CBCo	3	-7.135	-7.433	-1.000e-06	0.00542	0.556	0.823
tri_000_05827	NdPr	2	-4.687	-4.694	-2.900e-06	0.00216	0.11	0.116
tri_000_05829	NdPtSi	3	-6.394	-6.506	-3.000e-06	0.00266	0.201	0.12
tri_000_05856	LaSiYb	3	-3.594	-4.195	-7.000e-06	0.00392	0.526	0.425
tri_000_05870	CBMn	3	-7.674	-8.278	0.000e+00	0.00438	0.543	0.721
tri_000_05877	PtSn ₂ Yb	4	-4.328	-4.516	0.000e+00	0.00748	0.306	0.36
tri_000_05911	DyGd	2	-4.508	-4.548	-8.000e-07	0.00116	0.206	0.255
tri_000_05914	DyS ₂ Si	4	-4.788	-5.438	0.000e+00	0.00516	0.886	0.711
tri_000_05932	BeGeNd	3	-4.855	-4.965	-1.000e-06	0.00322	0.216	0.261
tri_000_06000	CoRu	2	-7.665	-7.963	-4.000e-06	0.00181	0.267	0.222
tri_000_06027	CaMnNdSb	4	-4.45	-4.827	-1.500e-05	0.00644	0.544	1.472
tri_000_06058	NiW	2	-8.723	-9.076	-9.000e-06	0.00979	0.326	0.162
tri_000_06066	Cl ₂ Dy	3	-4.505	-4.651	-1.000e-06	0.00374	0.351	0.404
tri_000_06073	AgRuZr	3	-6.185	-6.691	-3.000e-06	0.00688	0.44	0.533
tri_000_06080	RuZr	2	-8.549	-8.936	-6.000e-06	0.00832	0.379	0.235
tri_000_06087	NdTm	2	-4.545	-4.555	-1.420e-05	0.00085	0.063	0.069
tri_000_06105	NdTb	2	-4.548	-4.608	1.900e-06	0.00376	0.261	0.327
tri_000_06108	Ni ₂	2	-5.34	-5.384	-7.000e-06	0.00452	0.138	0.13
tri_000_06128	CoGeNd	3	-5.786	-5.926	0.000e+00	0.00529	0.242	0.358
tri_000_06145	AsPtTb	3	-5.99	-6.333	0.000e+00	0.00634	0.333	0.352
tri_000_06161	FeRe	2	-10.098	-10.25	6.000e-06	0.00181	0.242	0.203
tri_000_06172	DySe ₂	3	-4.812	-5.243	0.000e+00	0.00313	0.678	0.957
tri_000_06212	MnRe	2	-10.418	-10.601	1.000e-06	0.00497	0.219	0.222
tri_000_06247	MnZn	2	-4.742	-4.789	-7.900e-06	0.00503	0.12	0.081
tri_000_06257	CoIr	2	-7.522	-7.846	-2.600e-05	0.00875	0.222	0.161
tri_000_06275	NiRh	2	-6.077	-6.256	2.000e-06	0.00366	0.133	0.062
tri_000_06303	AuRu	2	-5.443	-5.756	-5.000e-06	0.00485	0.529	0.485
tri_000_06304	FePt	2	-6.748	-6.945	-9.000e-06	0.00355	0.285	0.288
tri_000_06320	GdGeTe	3	-4.174	-4.732	-1.000e-06	0.00661	1.272	0.542
tri_000_06339	PdSnYb	3	-4.026	-4.304	-1.000e-06	0.00522	0.657	0.738
tri_000_06352	DyGePt	3	-5.607	-6.115	0.000e+00	0.00462	1.116	0.718
tri_000_06399	AuNiTa	3	-5.868	-6.757	-7.000e-06	0.00587	0.35	0.329

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_06435	NiSn	2	-2.91	-4.605	-1.100e-05	0.00525	0.74	0.57
tri_000_06444	PtTeYb	3	-4.37	-4.635	-7.000e-06	0.00721	0.422	0.472
tri_000_06484	BeSiYb	3	-3.827	-3.89	0.000e+00	0.00124	0.161	0.194
tri_000_06487	CBTb	3	-6.387	-7.13	0.000e+00	0.00384	0.603	0.503
tri_000_06490	EuYb	2	-1.619	-1.641	9.000e-07	0.00067	0.161	0.255
tri_000_06496	Ag ₂ MnTh	4	-4.304	-4.703	6.000e-06	0.00421	0.553	0.578
tri_000_06498	B ₂ Ru	3	-7.207	-7.558	-1.000e-06	0.00276	0.465	0.628
tri_000_06499	AsNdSr	3	-4.117	-4.482	-7.000e-06	0.00664	0.588	0.97
tri_000_06501	GePTb	3	-3.605	-5.432	0.000e+00	0.0028	0.943	0.546
tri_000_06555	EuYb	2	-1.615	-1.641	-1.800e-06	0.00229	0.261	0.346
tri_000_06592	CBFe	3	-7.493	-7.85	-2.000e-06	0.00706	0.464	0.584
tri_000_06596	PtSnTb	3	-5.596	-5.826	-1.000e-06	0.00708	0.413	1.678
tri_000_06620	AsSiYb	3	-3.957	-4.288	-7.000e-06	0.00474	0.5	0.421
tri_000_06677	ErRu	2	-6.606	-6.841	-2.000e-05	0.00421	0.413	0.247
tri_000_06685	Pd ₂ Tb	3	-5.462	-5.742	0.000e+00	0.00297	0.955	0.692
tri_000_06701	GdSm	2	-4.54	-4.597	8.800e-06	0.00281	0.28	0.252
tri_000_06715	CoMo	2	-8.463	-8.766	-1.400e-05	0.00344	0.205	0.125
tri_000_06716	GeYbZn	3	-2.807	-2.91	-2.700e-05	0.00547	0.236	0.14
tri_000_06723	IrNi	2	-6.788	-7.105	-5.000e-06	0.00815	0.227	0.164
tri_000_06740	MnSe ₂	3	-5.051	-5.622	-1.000e-06	0.00522	0.492	0.617
tri_000_06746	AlDySi	3	-5.153	-5.167	0.000e+00	0.00292	0.073	0.069
tri_000_06763	AsDyPt	3	-5.493	-6.298	-1.000e-06	0.00443	0.881	0.617
tri_000_06786	Nd ₂	2	-4.671	-4.685	-2.000e-06	0.00125	0.123	0.078
tri_000_06800	AgAsTbTe	4	-4.089	-4.417	4.000e-06	0.00271	0.443	1.139
tri_000_06850	DyTm	2	-4.466	-4.503	-9.000e-07	0.00173	0.162	0.112
tri_000_06857	HNdO	3	-4.555	-5.497	-3.000e-06	0.00928	0.945	0.646
tri_000_06887	IrSb ₂ Yb	4	-5.242	-5.258	0.000e+00	0.00509	0.053	0.099
tri_000_06893	CuGdSe	3	-4.604	-4.751	-4.000e-06	0.00597	0.559	0.542
tri_000_06902	RuZr	2	-8.297	-8.902	5.000e-06	0.00629	0.39	0.197
tri_000_06928	NdTe	2	-5.186	-5.299	-1.000e-06	0.00465	0.303	0.141
tri_000_06937	CdNdZn	3	-2.098	-2.506	-2.490e-05	0.00727	0.811	0.679
tri_000_06950	NdS ₂	3	-5.19	-5.878	-2.000e-06	0.00337	1.564	1.033
tri_000_06958	B ₂ Ru	3	-7.106	-7.582	0.000e+00	0.00315	0.725	0.901
tri_000_06972	PTb	2	-6.225	-6.27	-1.000e-06	0.00211	0.142	0.149
tri_000_06975	AuTb	2	-4.49	-4.669	-6.600e-06	0.00107	0.199	0.237
tri_000_06980	NNdPt	3	-6.464	-7.208	-1.000e-06	0.0071	0.997	1.427
tri_000_06987	HfMn	2	-8.639	-9.224	-3.600e-05	0.00666	0.605	0.59
tri_000_07006	TbYb	2	-2.896	-2.907	-9.300e-06	0.00052	0.098	0.076
tri_000_07012	AuNi	2	-4.054	-4.141	9.000e-07	0.00358	0.211	0.311
tri_000_07030	CoMo	2	-8.366	-8.765	-4.200e-05	0.00453	0.367	0.425
tri_000_07060	MnPt	2	-7.385	-7.475	-2.000e-05	0.00399	0.173	0.164
tri_000_07083	FeZn ₂ Zr	4	-4.331	-4.507	9.000e-06	0.00462	0.494	0.995
tri_000_07126	AsMn ₂ Sb	4	-6.493	-6.614	2.000e-06	0.00734	0.38	0.413
tri_000_07133	EuYb	2	-1.632	-1.643	-1.200e-05	0.00149	0.177	0.108
tri_000_07135	DySe ₂	3	-3.811	-5.214	0.000e+00	0.00588	1.248	1.066
tri_000_07154	CuSeTb	3	-4.231	-4.726	0.000e+00	0.00274	0.816	0.805
tri_000_07165	MoNi	2	-7.965	-8.061	-1.300e-05	0.00706	0.107	0.185
tri_000_07175	AuNi	2	-4.071	-4.142	-9.500e-06	0.00511	0.138	0.103
tri_000_07196	MnZn	2	-4.658	-4.793	-5.900e-06	0.00079	0.292	0.225
tri_000_07211	Sb ₂ Tb	3	-4.428	-4.555	-3.000e-06	0.00256	0.989	1.193
tri_000_07259	TbZn	2	-2.82	-3.182	-1.500e-06	0.00131	0.846	0.66
tri_000_07270	IrNi	2	-6.712	-7.105	-4.900e-05	0.00682	0.169	0.101

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_07309	Br ₂ Yb	3	-2.7	-3.708	-7.000e-06	0.00597	0.303	0.727
tri_000_07314	MnV	2	-8.958	-9.136	-3.000e-05	0.00104	0.21	0.14
tri_000_07337	HBRu	3	-5.287	-6.14	2.000e-06	0.00839	0.524	1.497
tri_000_07353	AgSrTbTm	4	4.903	-3.226	-1.000e-06	0.00748	1.353	3.518
tri_000_07417	TbTe	2	-4.675	-5.137	-2.000e-06	0.00328	0.635	0.31
tri_000_07443	AcYb	2	-2.72	-2.73	3.100e-06	0.0055	0.129	0.084
tri_000_07448	ErNd	2	-4.565	-4.573	-1.720e-05	0.00343	0.067	0.045
tri_000_07506	FeNi	2	-6.595	-6.659	-3.000e-06	0.00357	0.103	0.064
tri_000_07560	Ru ₂ Se ₂	4	-4.705	-6.141	-8.000e-06	0.00522	0.514	0.985
tri_000_07574	TbY	2	-5.479	-5.494	-2.000e-06	0.00282	0.091	0.052
tri_000_07576	MoRu	2	-9.168	-10.002	-1.100e-05	0.0073	0.182	0.491
tri_000_07611	BiDyPdRh	4	-5.717	-5.741	-1.000e-06	0.00549	0.159	0.135
tri_000_07644	ScTb	2	-5.352	-5.363	-1.000e-06	0.00381	0.074	0.064
tri_000_07672	NiOs	2	-8.073	-8.194	0.000e+00	0.00563	0.135	0.123
tri_000_07680	DyTl	2	-3.564	-3.586	2.000e-07	0.00318	0.213	0.163
tri_000_07699	CBMn	3	-7.932	-8.278	-1.500e-05	0.00458	0.528	0.707
tri_000_07707	RuZr	2	-8.385	-8.912	-2.700e-05	0.00359	0.36	0.226
tri_000_07721	AsGeYb	3	-3.568	-4.114	8.000e-06	0.00459	0.429	0.434
tri_000_07748	GeInTb	3	-3.543	-4.34	-2.000e-06	0.00695	0.21	0.607
tri_000_07755	MnNi	2	-6.978	-7.15	-2.800e-05	0.00431	0.223	0.255
tri_000_07781	SbSiYb	3	-3.642	-3.962	-2.000e-06	0.00227	0.84	0.568
tri_000_07836	MnTc	2	-9.156	-9.494	-1.000e-06	0.00321	0.426	0.469
tri_000_07837	GdLiO	3	-3.613	-5.667	-5.000e-06	0.00605	0.716	0.411
tri_000_07850	H ₃ Mn	4	-3.576	-4.473	0.000e+00	0.00363	1.015	0.947
tri_000_07861	FeGa	2	-5.227	-5.522	0.000e+00	0.00362	0.377	0.379
tri_000_07913	PRuSi	3	-4.992	-6.752	-1.160e-04	0.00875	1.073	0.541
tri_000_07919	NiSn	2	-3.095	-4.575	-2.100e-06	0.00476	0.756	0.538
tri_000_07926	IrMn	2	-8.867	-9.049	-1.000e-05	0.00156	0.196	0.17
tri_000_07937	PtTeYb	3	-4.046	-4.631	-4.600e-05	0.00897	0.912	0.751
tri_000_08022	NdSn	2	-4.675	-4.953	-1.600e-06	0.00363	0.756	0.665
tri_000_08027	AgDyGa	3	-3.546	-3.881	1.000e-06	0.00565	0.415	1.606
tri_000_08050	PbYb	2	-2.883	-2.96	-2.000e-07	0.00301	0.221	0.147
tri_000_08058	Tb ₂	2	-4.538	-4.55	-1.700e-06	0.00113	0.11	0.082
tri_000_08059	NdPTe	3	-4.777	-5.346	-1.300e-05	0.00442	1.24	1.315
tri_000_08060	Tb ₂	2	-4.534	-4.55	-3.000e-07	0.00077	0.128	0.117
tri_000_08064	CLiMn	3	-6.187	-6.393	-2.000e-06	0.00755	0.261	0.284
tri_000_08067	BiNd	2	-4.807	-5.003	-1.000e-06	0.0023	0.791	0.649
tri_000_08081	Nd ₂	2	-4.657	-4.686	5.700e-06	0.00134	0.223	0.174
tri_000_08146	ErRu	2	-6.633	-6.889	-8.000e-06	0.00508	0.597	0.511
tri_000_08167	TbTm	2	-4.415	-4.506	3.000e-07	0.00051	0.241	0.247
tri_000_08173	Ni ₂	2	-5.358	-5.385	4.000e-06	0.0086	0.115	0.08
tri_000_08175	NiRu	2	-6.863	-7.187	0.000e+00	0.0035	0.237	0.223
tri_000_08192	NdRu	2	-6.117	-6.807	-1.900e-05	0.0072	0.876	0.857
tri_000_08195	Cl ₂ Dy	3	-4.24	-4.651	-1.000e-05	0.00527	0.427	0.505
tri_000_08210	CoRu	2	-7.367	-7.912	0.000e+00	0.00672	0.509	0.564
tri_000_08229	GePdYb	3	-4.259	-4.566	0.000e+00	0.00611	0.657	0.647
tri_000_08247	SbSrYb	3	-2.498	-3.028	-2.800e-06	0.00436	0.564	0.342
tri_000_08251	HfMn	2	-8.682	-9.228	-2.000e-06	0.00213	0.467	0.545
tri_000_08259	SeYb	2	-4.216	-4.398	-7.000e-07	0.00376	0.309	0.31
tri_000_08271	GaMn	2	-5.775	-5.847	2.000e-06	0.00199	0.165	0.138
tri_000_08285	HAuNaTb	4	-3.033	-3.329	0.000e+00	0.00504	1.238	0.386
tri_000_08287	BRuTi	3	-8.266	-8.342	-1.000e-06	0.0069	0.112	1.558

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_08345	BRuTb	3	-6.232	-7.233	-1.000e-06	0.00195	0.358	0.165
tri_000_08347	CoGdGe	3	-5.909	-5.942	1.000e-06	0.00585	0.157	0.101
tri_000_08385	DyPr	2	-4.599	-4.603	9.300e-06	0.00304	0.051	0.069
tri_000_08400	TbTe ₂	3	-4.519	-4.668	-1.000e-06	0.00441	0.657	0.88
tri_000_08420	GdSb	2	-4.712	-5.29	-1.000e-06	0.00078	0.584	0.584
tri_000_08431	HAsNiYb	4	-4.321	-4.462	-7.000e-06	0.00682	0.39	0.315
tri_000_08447	NdSm	2	-4.647	-4.654	5.200e-06	0.00295	0.085	0.109
tri_000_08473	GaGd	2	-3.97	-4.061	-1.240e-05	0.00351	0.386	0.392
tri_000_08482	NiPtTi	3	-6.675	-6.794	8.000e-06	0.00989	0.307	0.4
tri_000_08490	NdSiTe	3	-4.338	-4.942	-4.000e-06	0.00405	1.304	1.086
tri_000_08540	NdRh	2	-6.27	-6.356	-1.100e-05	0.00279	0.282	0.136
tri_000_08542	NiSbYb	3	-3.926	-4.369	-7.000e-06	0.00511	0.542	0.74
tri_000_08560	BeGeSYb	4	-3.979	-4.174	0.000e+00	0.0058	0.503	0.589
tri_000_08569	CuTb	2	-4.177	-4.188	-7.500e-06	0.00139	0.103	0.077
tri_000_08589	EuYb	2	-1.59	-1.642	-1.600e-05	0.00165	0.413	0.317
tri_000_08608	GeNdNiSe	4	-4.944	-5.233	-2.300e-05	0.0072	0.318	0.289
tri_000_08633	CoNi	2	-6.014	-6.054	-5.000e-06	0.00251	0.122	0.159
tri_000_08647	HGdTe	3	-3.592	-4.825	-2.000e-06	0.0045	1.618	2.976
tri_000_08648	GePdTb	3	-5.342	-5.726	-6.000e-05	0.00607	0.594	0.666
tri_000_08652	GaMn	2	-5.687	-5.848	-2.000e-06	0.00512	0.257	0.143
tri_000_08680	EuYb	2	-1.573	-1.641	-7.000e-07	0.00464	0.339	0.267
tri_000_08716	GdSiZn	3	-4.304	-4.356	-2.500e-05	0.00367	0.125	0.073
tri_000_08764	FeNi	2	-6.426	-6.658	-8.800e-05	0.00534	0.287	0.359
tri_000_08777	NiRu	2	-7.128	-7.194	-8.000e-06	0.00435	0.143	0.156
tri_000_08830	CSeTb	3	-5.197	-5.882	-8.000e-06	0.0021	0.551	0.541
tri_000_08843	CRuTh	3	-8.001	-8.815	-1.000e-06	0.00536	0.707	0.887
tri_000_08853	LaTb	2	-4.647	-4.679	-7.600e-06	0.00801	0.209	0.204
tri_000_08856	GdPtSe	3	-5.213	-5.843	0.000e+00	0.00521	0.971	0.797
tri_000_08872	NiZr	2	-6.796	-7.118	-1.100e-05	0.00591	0.837	0.626
tri_000_08926	DyO	2	-7.164	-7.417	0.000e+00	0.00511	0.18	0.084
tri_000_08939	HfNd	2	-6.689	-7.036	-1.400e-04	0.00496	0.415	0.188
tri_000_08945	MnPt	2	-6.963	-7.447	1.000e-06	0.00297	0.52	0.433
tri_000_08967	B ₂ Ru	3	-7.343	-7.434	0.000e+00	0.00434	0.318	0.214
tri_000_08970	PTlYb	3	-3.169	-3.643	0.000e+00	0.00405	0.474	0.424
tri_000_08994	HoTb	2	-4.516	-4.525	-5.000e-07	0.00231	0.075	0.029
tri_000_09000	RhRu	2	-8.173	-8.22	-5.000e-06	0.00129	0.102	0.115
tri_000_09052	NdY	2	-5.54	-5.549	-7.000e-06	0.00433	0.101	0.09
tri_000_09054	Co ₂	2	-6.727	-6.822	-2.000e-06	0.00612	0.203	0.234
tri_000_09062	GdSn ₂	3	-4.219	-4.477	-5.000e-06	0.00934	0.62	0.561
tri_000_09105	PtYbZn	3	-3.409	-3.724	-3.000e-06	0.00401	0.705	1.86
tri_000_09106	DyLiSe ₂	4	-4.982	-5.034	-7.000e-06	0.00712	0.215	0.212
tri_000_09116	H ₂ Mn	3	-4.01	-5.124	-1.000e-06	0.00197	0.242	1.477
tri_000_09155	AgNdSn	3	-3.24	-4.109	-1.000e-06	0.00348	0.492	1.8
tri_000_09158	SmTb	2	-4.526	-4.589	-1.000e-07	0.00228	0.284	0.365
tri_000_09167	GeNdSi	3	-5.384	-5.442	0.000e+00	0.0045	0.28	0.205
tri_000_09168	AsRuTe	3	-4.335	-5.587	-1.000e-06	0.00539	0.392	0.246
tri_000_09187	CTb	2	-5.512	-6.773	0.000e+00	0.00424	1.105	0.775
tri_000_09188	NaTb	2	-2.474	-2.689	-4.000e-07	0.00143	0.54	0.383
tri_000_09196	GdSc	2	-5.343	-5.37	-3.000e-06	0.00376	0.122	0.114
tri_000_09209	LuMn	2	-5.312	-5.983	3.000e-06	0.0066	0.705	0.556
tri_000_09238	GdO	2	-7.312	-7.409	0.000e+00	0.00282	0.177	0.128
tri_000_09249	HRuSi	3	-5.571	-6.057	0.000e+00	0.00598	0.162	0.792

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_09254	ErGd	2	-4.467	-4.531	1.210e-05	0.00525	0.196	0.133
tri_000_09284	B ₂ Ru	3	-7.359	-7.398	-1.000e-06	0.00422	0.088	0.107
tri_000_09382	DyHo	2	-4.495	-4.515	1.000e-06	0.00132	0.119	0.143
tri_000_09412	Tb ₂	2	-4.525	-4.548	0.000e+00	0.00135	0.159	0.189
tri_000_09421	NiZn	2	-3.34	-3.431	-1.000e-06	0.00239	0.216	0.156
tri_000_09447	GaGdSr	3	-2.694	-3.171	1.400e-06	0.00482	1.004	0.915
tri_000_09450	CoGdSn	3	-5.151	-5.506	-3.130e-04	0.00806	1.124	1.073
tri_000_09451	AgRhRu	3	-6.043	-6.173	0.000e+00	0.00444	0.234	0.238
tri_000_09462	SnYb	2	-2.816	-3.153	-2.300e-06	0.00617	0.571	0.63
tri_000_09491	AlDyPd	3	-5.079	-5.27	1.000e-06	0.00431	0.411	0.347
tri_000_09527	I ₂ Ru	3	-3.228	-3.975	-9.000e-06	0.00522	0.645	0.428
tri_000_09534	CoCr	2	-8.107	-8.171	3.000e-06	0.00508	0.137	0.221
tri_000_09580	Nd ₂	2	-4.654	-4.685	6.000e-06	0.00187	0.219	0.259
tri_000_09611	AcDy	2	-4.049	-4.204	-3.950e-05	0.00113	0.342	0.215
tri_000_09616	NdSi ₂	3	-0.443	-5.686	0.000e+00	0.00529	1.061	1.124
tri_000_09629	GdRhTe	3	-5.444	-5.962	0.000e+00	0.00101	1.001	0.815
tri_000_09643	NiPtTi	3	-6.652	-6.795	-3.000e-06	0.00897	0.268	0.28
tri_000_09656	GdY	2	-5.394	-5.506	-1.400e-05	0.0014	0.268	0.16
tri_000_09671	GdNaO	3	-4.621	-5.102	0.000e+00	0.00461	0.636	0.214
tri_000_09692	CuGaNd	3	-4.186	-4.238	4.000e-06	0.00296	0.199	0.155
tri_000_09710	CdNdSb	3	-3.513	-3.77	-1.000e-06	0.00295	0.822	0.802
tri_000_09723	ErGd	2	-4.501	-4.533	-7.600e-06	0.00991	0.126	0.073
tri_000_09739	DySi ₂	3	-5.636	-5.658	-1.000e-06	0.00301	0.186	0.129
tri_000_09744	CDyRu	3	-7.787	-7.828	-1.000e-06	0.00819	0.097	0.15
tri_000_09748	H ₂ Ni	3	-2.55	-4.007	-5.700e-05	0.00524	0.332	0.541
tri_000_09753	NdSm	2	-4.637	-4.654	3.400e-06	0.00201	0.105	0.114
tri_000_09770	MnPt	2	-7.055	-7.45	-1.000e-06	0.00034	0.53	0.507
tri_000_09839	Dy ₂	2	-4.47	-4.523	-2.000e-07	0.00029	0.219	0.14
tri_000_09906	NdSm	2	-4.647	-4.654	-4.300e-06	0.00291	0.105	0.078
tri_000_09913	I ₂ Yb	3	-3.049	-3.169	-1.700e-06	0.00229	0.382	0.233
tri_000_09915	FeTcZn	3	-6.233	-6.434	-3.000e-06	0.00727	0.201	0.154
tri_000_09936	HCrNi	3	-5.714	-6.067	-2.000e-06	0.00461	0.248	0.242
tri_000_09959	Ir ₂ MnMo	4	-9.167	-9.542	-3.000e-06	0.00454	0.377	1.06
tri_000_09974	ORbTb	3	-4.704	-4.982	1.000e-06	0.00986	0.747	0.451
tri_000_09976	YYb	2	-3.738	-3.839	-1.860e-05	0.0017	0.408	0.319
tri_000_09995	CoDy	2	-5.487	-5.907	-9.000e-06	0.00483	0.862	0.57
tri_000_10003	NdPr	2	-4.662	-4.693	-8.600e-06	0.00184	0.22	0.226
tri_000_10023	AlNi	2	-4.694	-5.08	1.000e-06	0.00165	0.435	0.488
tri_000_10039	BrSeTb	3	-5.02	-5.082	-1.000e-06	0.00653	0.149	0.143
tri_000_10081	Dy ₂	2	-4.501	-4.523	-3.400e-06	0.00177	0.118	0.112
tri_000_10160	AuNdSb	3	-4.472	-4.88	0.000e+00	0.00743	0.79	0.694
tri_000_10171	HfNi	2	-6.771	-7.805	0.000e+00	0.00702	0.898	0.659
tri_000_10195	Gd ₂	2	-4.564	-4.58	-8.000e-07	0.00398	0.097	0.095
tri_000_10200	MnSe	2	-5.155	-6.138	0.000e+00	0.00356	0.682	1.159
tri_000_10202	GaHoRu	3	-5.563	-5.952	0.000e+00	0.00809	1.119	0.92
tri_000_10246	CoNdP	3	-6.217	-6.679	0.000e+00	0.00476	0.516	0.637
tri_000_10252	BaSbYb	3	-0.624	-3.237	-1.170e-05	0.00566	1.068	0.648
tri_000_10254	BeSiYb	3	-3.811	-3.89	0.000e+00	0.00183	0.19	0.158
tri_000_10271	H ₂ Ni	3	-1.836	-3.958	0.000e+00	0.00203	0.428	0.427
tri_000_10320	NdNiSb	3	-5.474	-5.59	-7.200e-05	0.00803	0.139	0.344
tri_000_10328	GeSrTb	3	-3.509	-3.913	-4.000e-06	0.00684	0.498	0.358
tri_000_10355	DyLa	2	-4.577	-4.659	0.000e+00	0.0014	0.351	0.286

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_10357	GdTe	2	-5.057	-5.175	-2.000e-06	0.00468	0.216	0.123
tri_000_10397	CGeNd	3	-5.842	-6.064	-4.000e-06	0.00903	0.483	0.398
tri_000_10436	NbRu	2	-9.572	-9.787	-1.000e-06	0.00296	0.286	0.24
tri_000_10445	CBCoRu	4	-5.829	-7.771	-4.000e-06	0.00332	0.616	0.863
tri_000_10461	DySe ₂	3	-5.041	-5.243	0.000e+00	0.00316	0.564	0.508
tri_000_10474	CNd	2	-5.876	-6.384	-4.000e-06	0.00705	0.372	0.125
tri_000_10481	IrNi	2	-6.609	-7.105	-1.000e-06	0.00485	0.262	0.197
tri_000_10490	GdPtSr	3	-4.173	-4.765	-4.000e-06	0.00615	1.054	1.019
tri_000_10503	NbRu	2	-9.527	-9.692	-3.000e-06	0.00301	0.205	0.264
tri_000_10523	MnOsPd	3	-8.239	-8.363	-1.000e-06	0.00972	0.114	0.102
tri_000_10543	NdSb	2	-5.112	-5.384	0.000e+00	0.00523	0.561	0.509
tri_000_10558	CoRu	2	-7.571	-7.915	0.000e+00	0.00739	0.373	0.335
tri_000_10562	FeOsV	3	-9.197	-9.446	-3.000e-06	0.00244	0.391	0.484
tri_000_10566	CoMo	2	-8.388	-8.763	-3.700e-05	0.0007	0.233	0.19
tri_000_10583	GdYb	2	-2.914	-2.929	-3.600e-06	0.00369	0.124	0.077
tri_000_10622	Nd ₃ Sm	4	-0.708	-4.594	3.000e-06	0.00221	0.888	0.925
tri_000_10648	GdPtSe ₂	4	-5.298	-5.453	-2.000e-06	0.00489	0.461	1.488
tri_000_10653	B ₂ Ru	3	-7.233	-7.399	-2.000e-06	0.0055	0.182	0.114
tri_000_10671	CdNd	2	-2.731	-2.842	5.600e-06	0.00389	0.607	0.52
tri_000_10732	B ₂ Ru	3	-7.326	-7.433	-3.000e-06	0.00572	0.326	0.228
tri_000_10771	CGdTm	3	-6.243	-6.379	-1.000e-06	0.00662	0.293	0.45
tri_000_10778	GdNaO	3	-4.606	-5.097	-1.000e-06	0.00572	0.544	0.203
tri_000_10806	CoFeOs	3	-8.449	-8.589	-5.000e-06	0.00494	0.178	0.134
tri_000_10833	CuNi	2	-4.472	-4.592	6.000e-07	0.0019	0.488	0.209
tri_000_10851	NdSn	2	-4.622	-4.95	-2.000e-07	0.0067	0.718	0.551
tri_000_10859	NdSiTb	3	-4.863	-5.204	1.000e-06	0.00301	0.393	0.338
tri_000_10865	GePtYb	3	-4.729	-4.992	5.000e-06	0.00526	0.653	0.429
tri_000_10894	FeLuSi	3	-6.27	-6.493	-3.000e-06	0.00298	0.358	0.243
tri_000_10902	NdTe ₂	3	-4.542	-4.726	-3.000e-06	0.00587	0.937	1.109
tri_000_10913	FeRuTi	3	-8.015	-8.434	-1.000e-06	0.00449	0.417	0.426
tri_000_10933	TbTe ₂	3	-1.184	-4.659	-3.000e-06	0.00867	0.745	0.662
tri_000_10936	B ₂ Ru	3	-6.868	-7.401	-2.000e-06	0.00534	0.292	0.165
tri_000_10945	CGdNi	3	-6.235	-6.552	-7.000e-06	0.00584	0.41	0.493
tri_000_10949	GeNdSb	3	-4.346	-4.964	-2.000e-06	0.00751	0.771	0.679
tri_000_10965	FeSeZn	3	-4.106	-4.294	0.000e+00	0.00955	0.487	0.83
tri_000_10975	EuGd	2	-3.089	-3.112	-4.000e-07	0.00316	0.259	0.156
tri_000_10992	EuYb	2	-1.64	-1.642	-5.700e-06	0.00041	0.085	0.067
tri_000_11008	FeNbOs	3	-9.027	-9.818	-1.000e-06	0.00753	0.845	0.931
tri_000_11078	Br ₂ Dy	3	-3.816	-4.221	1.000e-06	0.00786	0.881	0.964
tri_000_11085	NiSn ₂	3	-3.796	-4.427	2.000e-06	0.00525	0.289	0.275
tri_000_11103	RhTb	2	-6.339	-6.628	1.000e-06	0.00109	0.505	0.558
tri_000_11106	PtTbTe	3	-5.215	-5.614	0.000e+00	0.00578	0.666	0.434
tri_000_11126	Tb ₂	2	-4.536	-4.551	-1.000e-07	0.00084	0.116	0.172
tri_000_11141	CrGdTe	3	-5.16	-5.575	-1.800e-05	0.00677	0.206	0.322
tri_000_11269	IrNaNd	3	-4.603	-4.837	1.000e-06	0.0085	0.404	2.647
tri_000_11284	DyGe ₂ Ni	4	-5.154	-5.195	1.000e-06	0.00565	0.304	0.262
tri_000_11312	DySV ₂	4	-6.272	-6.757	-3.900e-05	0.00465	0.774	0.735
tri_000_11328	MnRe	2	-10.325	-10.602	2.000e-06	0.00829	0.055	0.4
tri_000_11336	MnRh	2	-7.933	-8.132	-7.000e-06	0.00217	0.227	0.171
tri_000_11361	NSnTb	3	-5.886	-6.379	-3.000e-06	0.00752	0.612	0.829
tri_000_11415	GdNd	2	-4.607	-4.63	1.030e-05	0.00113	0.168	0.141
tri_000_11417	NdSi ₂	3	-5.654	-5.758	-4.000e-06	0.006	0.162	0.155

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_11446	AsBaTb	3	-3.856	-4.401	-5.000e-06	0.00311	0.394	0.236
tri_000_11459	DyTe	2	-4.641	-5.098	-4.000e-06	0.00205	0.587	0.386
tri_000_11470	DyPdSb	3	-5.11	-5.606	-2.000e-06	0.00738	0.881	0.939
tri_000_11489	NdSm	2	-4.646	-4.655	-1.500e-06	0.00511	0.077	0.054
tri_000_11495	AcDy	2	-4.143	-4.206	-7.000e-07	0.00131	0.256	0.203
tri_000_11498	AsPtTb	3	-6.159	-6.334	-1.000e-06	0.00683	0.301	0.201
tri_000_11499	AgNd	2	14.418	-3.603	-6.000e-07	0.00248	0.812	1.155
tri_000_11501	HGaNi	3	-3.457	-3.964	0.000e+00	0.00868	0.36	0.341
tri_000_11525	CoGeNd	3	-5.655	-5.924	0.000e+00	0.00566	0.669	0.661
tri_000_11529	CoNi	2	-6.038	-6.057	-1.700e-05	0.00448	0.08	0.088
tri_000_11535	SiTb	2	-5.184	-5.465	0.000e+00	0.00178	0.857	0.654
tri_000_11552	CaYb	2	-1.65	-1.686	-2.040e-05	0.002	0.219	0.267
tri_000_11555	PdSeTb	3	-5.071	-5.549	-6.000e-06	0.00929	1.014	2.284
tri_000_11568	DyLa	2	-4.545	-4.693	-2.000e-07	0.00349	0.712	0.64
tri_000_11569	AlCo	2	-5.411	-5.709	0.000e+00	0.00092	0.36	0.354
tri_000_11579	NdSn	2	-4.744	-4.747	-5.000e-07	0.00235	0.077	0.041
tri_000_11585	CoGdGe	3	-5.933	-5.942	-6.000e-06	0.00464	0.058	0.038
tri_000_11600	CuPTb	3	-5.561	-5.577	-3.400e-05	0.00858	0.078	0.051
tri_000_11631	HoRu	2	-6.399	-6.83	-9.000e-06	0.00518	0.357	0.515
tri_000_11665	FeIr	2	-8.47	-8.518	-1.100e-05	0.00345	0.107	0.162
tri_000_11713	F ₂ Yb	3	-5.643	-5.647	-2.000e-06	0.00518	0.032	0.026
tri_000_11716	Cu ₂ Gd	3	-4.164	-4.27	-2.000e-06	0.0016	0.211	0.268
tri_000_11743	GdNiPt	3	-5.764	-6.154	-1.000e-06	0.00565	0.641	0.574
tri_000_11747	GdMg	2	-2.913	-2.986	1.000e-07	0.00059	0.286	0.172
tri_000_11768	Co ₂ Li	3	-5.007	-5.068	0.000e+00	0.00504	0.285	0.34
tri_000_11780	IrNdSb	3	-6.498	-6.636	0.000e+00	0.00461	0.183	0.32
tri_000_11810	MnV ₂	3	-8.931	-9.111	-6.000e-06	0.00126	0.229	0.123
tri_000_11844	GdSiY	3	-5.697	-5.787	-6.000e-06	0.0034	0.429	0.357
tri_000_11861	DyLa	2	-4.585	-4.659	1.700e-06	0.00169	0.305	0.217
tri_000_11906	NiRe	2	-8.519	-8.877	-1.600e-05	0.00516	0.269	0.204
tri_000_11930	FeSbTeYb	4	-4.37	-4.668	-1.400e-05	0.00331	0.435	1.356
tri_000_11949	H ₂ Mn	3	-3.395	-5.099	-1.000e-06	0.00318	0.396	0.409
tri_000_11980	RuSW	3	-8.174	-8.834	-2.000e-06	0.00668	0.521	0.602
tri_000_11993	DyTb	2	-4.491	-4.536	-3.000e-07	0.00076	0.201	0.203
tri_000_11998	NdPr	2	-4.664	-4.694	1.570e-05	0.00088	0.206	0.177
tri_000_12079	Co ₂ SiTb	4	-6.031	-6.08	-6.000e-06	0.00968	0.125	0.143
tri_000_12104	BeSiYb	3	-3.884	-3.891	0.000e+00	0.00185	0.052	0.036
tri_000_12109	GdTb	2	-4.545	-4.559	-3.100e-06	0.00357	0.098	0.08
tri_000_12113	Be ₂ DyGe	4	9.084	-4.208	0.000e+00	0.00513	0.836	1.281
tri_000_12119	CoW	2	-9.274	-9.785	-7.000e-05	0.0061	0.344	0.2
tri_000_12136	PSiTb	3	-5.684	-5.752	0.000e+00	0.00314	0.256	0.309
tri_000_12178	GdY	2	-5.479	-5.505	1.000e-06	0.00059	0.144	0.155
tri_000_12181	MgNd	2	-3.026	-3.054	9.000e-06	0.00125	0.199	0.131
tri_000_12184	PtRuZn	3	-4.951	-5.53	1.000e-06	0.00536	0.183	0.316
tri_000_12245	NiSiYb	3	-3.647	-4.64	2.000e-06	0.00681	0.661	0.842
tri_000_12255	FeRe	2	-10.018	-10.25	-3.000e-06	0.00739	0.226	0.141
tri_000_12258	CoPdRu	3	-6.666	-6.947	-6.000e-06	0.00865	0.4	0.411
tri_000_12265	AuNi	2	-3.765	-4.132	-9.000e-07	0.00389	0.278	0.154
tri_000_12292	SnYb	2	-2.775	-3.158	-1.000e-07	0.00505	0.565	0.725
tri_000_12344	CuNi	2	-4.532	-4.573	-2.900e-06	0.00359	0.133	0.108
tri_000_12363	OsRu	2	-9.402	-10.092	1.200e-05	0.00523	0.474	0.541
tri_000_12380	DyOSb	3	-5.838	-6.476	-1.000e-06	0.00828	0.447	1.064

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_12383	DyTe	2	4.789	-5.065	0.000e+00	0.00526	1.813	2.443
tri_000_12409	CoDyGe	3	-5.937	-5.935	-7.000e-06	0.00416	0.16	0.2
tri_000_12444	PrTb	2	-4.592	-4.618	-2.000e-06	0.0009	0.127	0.123
tri_000_12450	CoOs	2	-8.744	-8.992	-7.000e-06	0.00745	0.168	0.143
tri_000_12483	DyPtS ₂	4	-5.659	-5.856	-1.400e-05	0.00481	0.612	1.648
tri_000_12497	NdSm	2	-4.635	-4.654	8.500e-06	0.00358	0.17	0.2
tri_000_12533	IrMoNi	3	-7.868	-8.424	-4.300e-05	0.00745	0.352	0.27
tri_000_12560	MnZn	2	-4.639	-4.79	-5.000e-07	0.00061	0.281	0.155
tri_000_12619	CoPt	2	-6.33	-6.361	-2.000e-06	0.00587	0.093	0.104
tri_000_12647	MnS ₂	3	-5.98	-6.05	-2.400e-05	0.00345	0.164	0.103
tri_000_12648	AsCrNd	3	-6.124	-6.565	-6.000e-06	0.00286	0.787	0.681
tri_000_12653	NbRu	2	-8.787	-9.761	-2.000e-06	0.00228	0.263	0.199
tri_000_12669	RhTbTe	3	-5.395	-5.971	-4.000e-06	0.00544	0.703	0.758
tri_000_12691	LuNd	2	-4.451	-4.539	6.900e-06	0.00103	0.276	0.205
tri_000_12700	HMnTb	3	-5.031	-5.402	0.000e+00	0.00891	0.635	1.602
tri_000_12707	NiRh	2	-6.07	-6.252	0.000e+00	0.00659	0.127	0.074
tri_000_12713	Co ₂	2	-6.764	-6.822	-7.000e-06	0.0072	0.135	0.162
tri_000_12727	NbRuTa	3	-9.982	-10.509	0.000e+00	0.00447	0.363	0.193
tri_000_12743	FeMnPt	3	-7.518	-7.677	0.000e+00	0.00387	0.261	0.23
tri_000_12766	DySe ₂	3	-4.842	-5.236	0.000e+00	0.00233	0.841	1.182
tri_000_12791	CoPt	2	-5.917	-6.399	0.000e+00	0.0018	0.529	0.263
tri_000_12801	AgDyTe ₂	4	-4.041	-4.281	-2.000e-06	0.00396	0.367	0.289
tri_000_12859	FeZn	2	-4.365	-4.412	2.100e-06	0.00449	0.152	0.181
tri_000_12869	GdSi ₂	3	-5.676	-5.701	0.000e+00	0.00516	0.194	0.126
tri_000_12873	Br ₂ Nd	3	-4.169	-4.343	1.000e-06	0.00682	0.364	0.414
tri_000_12876	LiS ₂ Tb	4	-5.055	-5.527	-1.000e-06	0.0053	0.486	0.634
tri_000_12900	MnSnTe	3	-5.023	-5.074	0.000e+00	0.00506	0.129	0.144
tri_000_12921	FePtV	3	-7.583	-7.859	-2.000e-06	0.00517	0.197	0.307
tri_000_12953	AuNi	2	-3.547	-4.129	0.000e+00	0.00329	0.239	0.12
tri_000_12960	DySeTa	3	-6.685	-7.079	-1.000e-06	0.00181	0.363	0.421
tri_000_12963	GdTb	2	-4.553	-4.561	-9.000e-07	0.00107	0.089	0.062
tri_000_12995	Cl ₂ Yb	3	-4.168	-4.202	0.000e+00	0.00306	0.274	0.389
tri_000_13032	DyGeTb	3	-4.667	-4.974	1.000e-06	0.00472	0.94	0.709
tri_000_13040	Co ₂	2	-6.806	-6.822	3.000e-06	0.00561	0.065	0.041
tri_000_13042	GdHo	2	-4.496	-4.539	-1.100e-06	0.00205	0.194	0.111
tri_000_13077	RuTi	2	-8.813	-8.92	-2.900e-05	0.0052	0.143	0.087
tri_000_13078	RuZn	2	-4.962	-5.071	0.000e+00	0.00788	0.535	0.293
tri_000_13155	As ₂ DyFe	4	-5.92	-6.14	1.000e-06	0.00448	0.329	1.119
tri_000_13158	MnOs	2	-9.876	-10.106	1.000e-06	0.00134	0.194	0.252
tri_000_13194	Se ₂ Tb	3	-4.846	-5.252	-1.000e-06	0.00319	0.598	0.791
tri_000_13208	GdP	2	-2.856	-6.06	0.000e+00	0.00717	0.79	0.644
tri_000_13234	DyGd	2	-4.517	-4.546	-6.400e-06	0.00222	0.122	0.081
tri_000_13265	CMnV	3	-8.807	-9.287	-1.000e-06	0.00641	0.453	1.373
tri_000_13272	NdPtSb	3	-5.244	-6.045	2.000e-06	0.00701	1.006	0.757
tri_000_13312	PYYb	3	-4.964	-5.346	-1.000e-06	0.00415	0.456	0.571
tri_000_13331	MnZn ₂	3	-3.477	-3.53	0.000e+00	0.004	0.153	0.158
tri_000_13335	GeNdZn	3	-3.861	-4.128	1.000e-06	0.00853	0.229	1.722
tri_000_13349	CDy ₂	3	-6.186	-6.364	-1.000e-06	0.00284	0.277	0.345
tri_000_13367	AuMn	2	-5.197	-5.492	-1.000e-06	0.00146	0.516	0.431
tri_000_13374	MnZn	2	-4.368	-4.804	3.000e-07	0.00279	0.434	0.151
tri_000_13377	CDyGa	3	-5.637	-5.725	0.000e+00	0.00547	0.182	0.266
tri_000_13399	NdTh	2	-5.929	-6.005	-5.000e-06	0.00108	0.298	0.294

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_13411	AcNd	2	-4.316	-4.335	2.300e-06	0.00319	0.16	0.153
tri_000_13448	CdCo	2	-2.702	-3.338	3.000e-07	0.00399	0.587	0.427
tri_000_13452	CoOs	2	-8.464	-8.989	1.000e-06	0.0019	0.301	0.209
tri_000_13460	STeYb	3	-3.476	-4.054	0.000e+00	0.00275	1.301	2.964
tri_000_13464	AlNNd	3	-5.889	-6.159	1.000e-06	0.00612	0.6	0.572
tri_000_13566	AuTbTm	3	-4.09	-4.469	-4.000e-06	0.00544	0.733	0.763
tri_000_13587	FeNbPd	3	-7.617	-7.818	0.000e+00	0.00947	0.687	0.409
tri_000_13589	MnMoOs	3	-9.784	-10.152	-1.500e-05	0.00585	0.385	0.363
tri_000_13601	CoMnV	3	-8.102	-8.336	-1.100e-05	0.00466	0.435	0.414
tri_000_13646	AsCrTb	3	-6.122	-6.558	1.000e-06	0.00968	0.678	0.683
tri_000_13650	HALSiYb	4	-3.13	-3.571	-1.000e-06	0.00479	0.453	1.196
tri_000_13678	NiPd	2	-5.103	-5.198	0.000e+00	0.00259	0.17	0.156
tri_000_13720	BeDySi	3	-5.19	-5.226	-4.000e-06	0.00513	0.119	0.084
tri_000_13723	NdTe ₂	3	-4.6	-4.619	1.000e-06	0.00106	0.406	0.36
tri_000_13740	DyMnTe	3	-5.347	-5.78	-1.000e-06	0.00727	1.038	1.128
tri_000_13747	BCoSb	3	-5.45	-5.533	1.000e-06	0.0039	0.329	0.4
tri_000_13756	C ₂ Tb	3	-6.808	-7.846	-1.000e-06	0.00703	0.593	0.539
tri_000_13757	AlCo	2	-5.467	-5.709	0.000e+00	0.00296	0.277	0.231
tri_000_13764	NiRh	2	-6.249	-6.271	-2.000e-06	0.00471	0.078	0.109
tri_000_13789	HBRu	3	-5.794	-6.344	-1.000e-06	0.00338	0.255	0.733
tri_000_13797	AgCuHgNd	4	-2.876	-3.029	-1.100e-05	0.00364	0.27	1.426
tri_000_13815	NdSSe	3	-5.059	-5.522	0.000e+00	0.0027	0.731	0.663
tri_000_13840	CeYb	2	-3.27	-3.445	4.000e-07	0.00138	0.557	0.655
tri_000_13849	CoSi	2	-6.222	-6.606	-1.800e-05	0.00964	0.453	0.51
tri_000_13869	PrTb	2	-4.566	-4.612	2.110e-05	0.00492	0.218	0.153
tri_000_13876	NiZn	2	-3.336	-3.431	-1.600e-06	0.00768	0.214	0.224
tri_000_13922	CoNdSb	3	-5.664	-5.848	-1.000e-06	0.00808	0.452	1.799
tri_000_13957	FeGdSe	3	-5.574	-6.085	-1.000e-05	0.00907	0.806	0.737
tri_000_13976	DyTb	2	-4.519	-4.541	4.000e-07	0.00317	0.136	0.055
tri_000_13986	DyTm	2	-4.483	-4.497	1.000e-06	0.00214	0.083	0.059
tri_000_13996	MnOs	2	-9.823	-10.111	2.000e-06	0.0045	0.237	0.312
tri_000_14026	NdPtSi	3	-6.016	-6.51	-1.000e-06	0.006	0.404	0.259
tri_000_14045	AsSiTb	3	-3.651	-5.412	-3.000e-06	0.00347	0.891	0.757
tri_000_14051	CTb	2	-5.298	-6.745	1.000e-06	0.00385	1.164	1.03
tri_000_14068	NSbTb	3	-5.758	-6.381	0.000e+00	0.00628	0.533	0.61
tri_000_14073	HTb	2	-4.041	-4.342	-6.000e-06	0.00208	0.999	0.59
tri_000_14074	GdNiSb	3	-4.867	-5.541	-1.000e-05	0.00399	0.899	0.704
tri_000_14080	CNiTm	3	-6.179	-6.585	-1.620e-04	0.00651	0.584	1.866
tri_000_14122	CrGdSe	3	-5.746	-6.029	0.000e+00	0.00478	0.293	0.321
tri_000_14157	TbTm	2	-4.501	-4.511	2.000e-07	0.00236	0.022	0.034
tri_000_14203	GeOsYb	3	-5.589	-5.914	3.000e-06	0.00603	0.517	0.628
tri_000_14235	RuS ₂	3	-5.891	-6.034	-2.000e-06	0.00442	0.509	0.292
tri_000_14269	AlCo	2	-5.634	-5.713	-2.600e-05	0.00459	0.18	0.169
tri_000_14326	LuRu	2	-6.215	-6.848	-1.800e-05	0.00698	0.482	0.398
tri_000_14331	DyRhTe	3	-5.086	-5.796	2.000e-06	0.00436	1.045	0.785
tri_000_14346	AlEuNd	3	-3.193	-3.549	1.000e-06	0.00376	1.036	2.413
tri_000_14360	LuNdTb	3	-4.538	-4.554	1.000e-06	0.0036	0.25	0.197
tri_000_14373	CGeTb	3	-5.888	-5.95	1.000e-06	0.00504	0.362	0.439
tri_000_14379	NdRhSn	3	-5.839	-5.971	-5.000e-06	0.00985	0.426	1.907
tri_000_14383	H ₂ Yb	3	-2.247	-3.281	-2.060e-05	0.00203	0.348	0.709
tri_000_14389	CoTc	2	-8.436	-8.602	1.400e-05	0.00973	0.137	0.091
tri_000_14412	AsGd	2	-5.597	-5.869	-1.000e-06	0.00209	0.375	0.286

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_14419	CeGd	2	-5.121	-5.139	3.000e-06	0.00847	0.165	0.132
tri_000_14436	CeSiTb	3	-4.605	-5.606	3.000e-06	0.00448	0.948	0.698
tri_000_14482	AlMn	2	-6.274	-6.396	-2.000e-06	0.00621	0.324	0.191
tri_000_14489	CAIBMn	4	-6.221	-7.01	-1.000e-06	0.00382	0.685	0.57
tri_000_14515	NdNiSi	3	-5.907	-5.913	-2.370e-04	0.00989	0.067	0.054
tri_000_14542	CoRh	2	-6.832	-6.964	-8.000e-06	0.00898	0.169	0.153
tri_000_14592	NiZn	2	-3.354	-3.432	2.000e-07	0.00906	0.173	0.089
tri_000_14652	FeOs	2	-9.282	-9.648	-1.600e-05	0.00339	0.258	0.178
tri_000_14680	Nd ₂	2	-4.679	-4.686	3.700e-06	0.00223	0.103	0.092
tri_000_14685	BrRuS	3	-4.612	-5.247	-1.000e-06	0.00843	0.665	0.806
tri_000_14691	FeNdTe	3	-5.22	-5.774	6.000e-06	0.0089	1.149	0.829
tri_000_14694	FeRh ₂	3	-7.405	-7.482	-3.000e-06	0.00496	0.151	0.2
tri_000_14739	CrGdTe	3	-5.256	-5.816	-2.000e-06	0.00586	0.898	0.744
tri_000_14777	GdSm	2	-4.597	-4.6	-2.000e-07	0.00069	0.047	0.055
tri_000_14789	DyEu	2	-3.031	-3.068	4.000e-07	0.00248	0.257	0.279
tri_000_14822	HSiYb	3	-3.228	-3.557	1.000e-06	0.00421	0.717	0.801
tri_000_14830	DySb ₂	3	-4.221	-4.908	-1.200e-05	0.00861	1.338	0.74
tri_000_14843	AsDyPt ₂	4	-5.67	-6.105	0.000e+00	0.00309	0.944	0.958
tri_000_14889	AuDyNiV	4	-4.961	-5.756	-6.000e-06	0.00739	0.433	0.464
tri_000_14913	ErNd	2	-4.526	-4.569	-9.900e-06	0.00733	0.214	0.271
tri_000_14917	PrTb	2	-4.599	-4.618	4.100e-06	0.00176	0.104	0.062
tri_000_14956	Tb ₂	2	-0.386	-4.283	-8.340e-05	0.00397	0.908	0.526
tri_000_14979	AsPt ₂ Yb	4	-4.981	-5.272	-2.000e-06	0.00624	0.799	0.702
tri_000_15005	MnZn ₃	4	-2.846	-2.932	-1.000e-06	0.00711	0.329	2.619
tri_000_15013	H ₂ BF _e	4	-4.021	-5.117	0.000e+00	0.0042	0.549	1.299
tri_000_15036	GdGePSr	4	-3.977	-4.331	-2.000e-06	0.00481	0.599	0.562
tri_000_15048	NdZn	2	-2.904	-2.955	-1.440e-05	0.00383	0.157	0.191
tri_000_15061	AuGeYb	3	-3.325	-3.875	-3.600e-05	0.00777	1.096	1.145
tri_000_15075	H ₂ Co	3	-2.736	-4.473	-2.000e-06	0.00352	0.435	1.093
tri_000_15083	InMn	2	-4.484	-5.032	1.089e-01	0.00407	0.511	0.501
tri_000_15151	Si ₂ Yb	3	-4.414	-4.46	-1.300e-05	0.00158	0.137	0.085
tri_000_15154	B ₂ Ru	3	-6.158	-7.603	-2.000e-06	0.00357	0.614	0.393
tri_000_15179	GdS ₂	3	-5.239	-5.836	-9.000e-06	0.00434	1.42	1.338
tri_000_15201	CBeRu	3	-6.649	-7.144	-2.000e-06	0.0054	0.783	0.63
tri_000_15254	EuYb	2	-1.564	-1.642	-2.600e-06	0.00465	0.461	0.334
tri_000_15258	DySb ₂ Ti	4	-5.228	-5.869	-1.200e-05	0.00368	0.471	0.392
tri_000_15274	FeZn	2	-4.334	-4.414	2.000e-06	0.00444	0.154	0.308
tri_000_15281	FeRu	2	-8.297	-8.606	0.000e+00	0.00462	0.358	0.309
tri_000_15285	CdYb	2	-1.294	-1.331	-2.940e-05	0.00325	0.176	0.259
tri_000_15311	PtSb ₂ Yb	4	-4.272	-4.668	2.000e-06	0.00438	0.354	0.334
tri_000_15312	ReRu	2	-10.749	-10.895	-2.000e-06	0.0036	0.131	0.149
tri_000_15348	CuGaTb	3	-4.127	-4.24	-6.600e-05	0.00994	0.348	0.359
tri_000_15363	NdSiZn	3	-4.193	-4.392	-2.000e-06	0.00377	0.182	0.33
tri_000_15365	CuNi	2	-4.565	-4.575	-1.400e-05	0.00665	0.08	0.064
tri_000_15368	CoMo	2	-8.356	-8.763	-2.400e-05	0.00485	0.301	0.215
tri_000_15380	GdPt ₂ Yb	4	-5.678	-5.731	-1.000e-06	0.00515	0.207	0.159
tri_000_15387	Ba ₂ Nd	3	-2.339	-2.659	6.100e-06	0.00285	0.728	0.743
tri_000_15391	TbTm	2	-4.506	-4.511	3.000e-07	0.00473	0.059	0.055
tri_000_15398	Br ₂ Nd	3	-4.195	-4.343	3.600e-05	0.00737	0.457	0.519
tri_000_15456	BrPtYb	3	-3.247	-3.769	-8.000e-06	0.00446	1.755	3.537
tri_000_15462	NiSeYb	3	-4.208	-4.575	-1.700e-05	0.00478	0.394	0.602
tri_000_15593	FeGdPSi	4	4.85	-6.402	0.000e+00	0.00562	1.035	1.186

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_15606	CuGdP	3	-4.971	-5.589	-1.000e-05	0.0036	0.58	1.918
tri_000_15629	NdPtSb	3	-5.661	-6.073	-4.000e-06	0.00402	0.673	0.853
tri_000_15634	GePTb	3	-5.121	-5.435	0.000e+00	0.00812	0.49	0.407
tri_000_15649	FePt	2	-6.687	-6.964	2.000e-06	0.00365	0.277	0.261
tri_000_15674	CoDySi	3	-6.009	-6.29	-1.000e-05	0.00803	0.565	0.52
tri_000_15678	B ₂ Ru	3	-7.207	-7.586	0.000e+00	0.00631	0.771	0.498
tri_000_15688	Ni ₂	2	-5.299	-5.384	-2.900e-05	0.00667	0.185	0.177
tri_000_15704	H ₂ Co	3	-4.279	-4.487	-2.000e-06	0.00353	0.282	0.306
tri_000_15714	AuNi	2	-4.089	-4.139	-1.070e-05	0.00452	0.133	0.108
tri_000_15719	RhRu	2	-7.605	-8.156	1.500e-05	0.00491	0.387	0.321
tri_000_15721	IrMn	2	-9.005	-9.054	-5.900e-05	0.00748	0.089	0.047
tri_000_15728	MnRu	2	-8.928	-9.069	-8.000e-06	0.00356	0.173	0.191
tri_000_15784	FeOs	2	-9.054	-9.531	-1.000e-06	0.00291	0.505	0.328
tri_000_15792	GaSi ₂ Tb	4	7.54	-4.63	-1.100e-05	0.0073	1.048	1.187
tri_000_15817	TbTm	2	-4.44	-4.508	-4.000e-07	0.0017	0.245	0.222
tri_000_15820	GdPd	2	-5.522	-5.55	-1.000e-06	0.00251	0.179	0.187
tri_000_15839	NaSiTb	3	-2.514	-3.816	0.000e+00	0.0033	0.883	0.847
tri_000_15852	DyHo	2	-4.504	-4.518	-6.440e-05	0.00824	0.113	0.119
tri_000_15858	GdHo	2	-4.519	-4.54	-1.180e-05	0.00196	0.13	0.124
tri_000_15880	CrTeYb	3	-4.098	-4.483	-1.100e-05	0.00925	0.958	1.153
tri_000_15892	NiSeYb	3	-4.12	-4.575	8.000e-06	0.00252	0.384	0.625
tri_000_15899	NdS ₂	3	-5.428	-5.881	-3.000e-06	0.00579	1.271	1.416
tri_000_15915	NbNdTe	3	-5.922	-6.174	-1.000e-06	0.00353	0.259	0.25
tri_000_15927	NiZn	2	-3.235	-3.44	-1.120e-05	0.00409	0.292	0.46
tri_000_15935	NdTe	2	-5.2	-5.303	-3.000e-06	0.00335	0.216	0.123
tri_000_15941	CoNi	2	-5.937	-6.056	-2.100e-05	0.00914	0.273	0.29
tri_000_15953	AuDyI	3	-3.574	-3.848	0.000e+00	0.00496	0.573	0.623
tri_000_15985	FePt	2	-6.879	-6.947	2.000e-06	0.00308	0.16	0.147
tri_000_15996	IrRu	2	-8.968	-9.079	-1.500e-05	0.00436	0.163	0.22
tri_000_16012	AlGdSi	3	-5.205	-5.215	-1.000e-06	0.00353	0.05	0.034
tri_000_16016	FeNbTi	3	-7.967	-8.73	-3.000e-06	0.0062	0.528	0.506
tri_000_16102	DyS ₂	3	-5.263	-5.794	0.000e+00	0.00451	1.678	1.666
tri_000_16117	CoO ₂ Zr	4	-7.62	-8.034	3.000e-06	0.00648	0.374	0.305
tri_000_16131	AlFe	2	-5.782	-6.133	0.000e+00	0.00558	0.291	0.436
tri_000_16147	FeMo ₂	3	-9.496	-9.851	3.000e-06	0.00465	0.579	0.396
tri_000_16161	AlGdSe ₂	4	-4.714	-4.88	1.000e-06	0.00295	0.578	1.268
tri_000_16178	DySe ₂	3	-4.916	-5.235	0.000e+00	0.00419	0.839	0.846
tri_000_16195	RhRu	2	-8.057	-8.22	0.000e+00	0.00208	0.147	0.106
tri_000_16206	DySe ₂	3	-4.858	-5.226	0.000e+00	0.00335	1.074	0.828
tri_000_16220	Tb ₂	2	-4.505	-4.55	-1.100e-06	0.00374	0.239	0.145
tri_000_16227	Ni ₂ Ta	3	-7.027	-7.572	5.848e-02	0.00922	0.736	0.505
tri_000_16265	GdTe	2	-4.906	-5.174	0.000e+00	0.0012	0.472	0.465
tri_000_16284	H ₂ Mn	3	4.252	-4.176	-5.000e-06	0.00632	0.425	1.105
tri_000_16343	AgMn	2	-4.68	-5.081	1.000e-06	0.00076	0.493	0.499
tri_000_16385	NiPd	2	-5.035	-5.196	2.000e-06	0.00038	0.152	0.072
tri_000_16407	CaGeTb	3	-3.747	-3.964	-5.000e-06	0.00378	0.413	0.306
tri_000_16408	GdSb ₂ Ti	4	-5.564	-5.89	-1.200e-05	0.00711	0.326	0.233
tri_000_16412	LuNd	2	-4.497	-4.54	3.200e-06	0.00108	0.205	0.096
tri_000_16417	DyYb	2	-2.726	-2.883	7.600e-06	0.00218	0.499	0.308
tri_000_16420	GdNd	2	-4.596	-4.63	7.000e-07	0.00244	0.2	0.162
tri_000_16461	NdRuSi	3	-6.862	-7.018	-1.100e-05	0.00422	0.232	1.466
tri_000_16472	GdPt ₂ Sb	4	-5.715	-6.087	-2.000e-06	0.00214	0.531	0.475

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_16473	NdO	2	-6.898	-7.284	1.000e-06	0.00612	0.411	0.438
tri_000_16506	Gd ₂ Pd	3	-5.131	-5.202	-4.000e-06	0.00431	0.289	0.346
tri_000_16521	DySe ₂	3	-5.062	-5.242	-4.000e-06	0.00514	1.048	0.495
tri_000_16530	DyNd	2	-4.587	-4.599	5.000e-07	0.00186	0.108	0.047
tri_000_16598	CrSTb	3	-5.966	-6.537	8.000e-06	0.00972	0.31	0.473
tri_000_16622	CGd ₂	3	-6.007	-6.352	0.000e+00	0.00492	0.686	0.674
tri_000_16631	Gd ₂ Te ₂	4	-5.135	-5.216	0.000e+00	0.00281	0.284	0.258
tri_000_16672	CoMn	2	-7.86	-7.984	-1.000e-05	0.00232	0.125	0.065
tri_000_16697	Cd ₃ Gd	4	-1.481	-1.975	-1.800e-06	0.00284	0.531	0.305
tri_000_16705	MnOs	2	-9.998	-10.109	1.000e-06	0.00203	0.143	0.124
tri_000_16716	CoMoPt	3	-7.283	-7.954	-1.800e-05	0.0088	0.242	0.145
tri_000_16727	NdTb	2	-4.507	-4.628	-1.800e-06	0.00198	0.715	0.474
tri_000_16753	FeIr	2	-8.256	-8.517	1.000e-06	0.00292	0.292	0.197
tri_000_16787	ErTb	2	-4.508	-4.518	2.940e-05	0.00589	0.097	0.067
tri_000_16798	Be ₂ Dy	3	-3.813	-3.947	-2.100e-05	0.00064	0.353	0.226
tri_000_16809	DyGaPr	3	-3.306	-4.312	-6.000e-06	0.00325	0.866	0.637
tri_000_16822	EuTb	2	-3.085	-3.094	9.000e-07	0.00206	0.088	0.163
tri_000_16832	NiPt	2	-5.427	-5.752	-3.600e-05	0.00408	0.271	0.186
tri_000_16838	LiRu	2	-4.988	-5.387	-2.000e-06	0.00455	0.374	0.337
tri_000_16860	IrRu	2	-8.747	-9.079	-2.000e-06	0.0061	0.315	0.296
tri_000_16956	GeNdSb	3	-4.884	-4.968	0.000e+00	0.0031	0.223	0.137
tri_000_16962	AlDyGd	3	-3.392	-4.434	-3.000e-06	0.00128	0.897	0.753
tri_000_16988	MnOsRh	3	-8.778	-9.098	-2.000e-06	0.00533	0.324	0.382
tri_000_16995	HBeMnRu	4	-5.739	-6.184	-2.000e-06	0.00478	0.496	0.639
tri_000_17000	Ge ₂ Yb	3	-3.817	-3.954	-1.000e-06	0.0088	0.348	0.284
tri_000_17008	RuSc	2	-7.758	-7.934	-1.000e-06	0.0048	0.4	0.304
tri_000_17059	AuGdSb	3	-4.434	-4.8	-1.000e-06	0.00496	0.63	0.411
tri_000_17064	PmRu	2	-5.617	-6.563	-2.100e-05	0.00456	0.581	0.598
tri_000_17077	IPtYb	3	-3.345	-3.594	0.000e+00	0.00982	0.945	0.847
tri_000_17082	Tb ₂	2	-4.534	-4.547	-2.200e-06	0.00154	0.105	0.046
tri_000_17089	DySe	2	-5.667	-5.672	0.000e+00	0.00257	0.045	0.029
tri_000_17100	GdTm	2	-4.495	-4.517	-5.100e-06	0.00092	0.116	0.153
tri_000_17146	PtRu	2	-7.194	-7.533	-3.600e-05	0.00307	0.243	0.19
tri_000_17158	EuYb	2	-1.622	-1.642	-1.400e-06	0.0021	0.185	0.252
tri_000_17196	AsRuSeV	4	-6.512	-6.795	1.000e-06	0.00693	0.28	0.278
tri_000_17251	AlSiYb	3	-3.893	-3.943	-1.300e-05	0.00395	0.184	0.148
tri_000_17252	HoNd	2	-4.574	-4.585	-1.600e-06	0.00384	0.119	0.066
tri_000_17254	DySiSr	3	-3.611	-4.05	0.000e+00	0.00374	0.52	0.313
tri_000_17264	NiTc	2	-7.542	-7.841	-1.870e-04	0.00892	0.366	0.309
tri_000_17273	MnRh	2	-8.093	-8.128	-1.000e-06	0.00761	0.089	0.095
tri_000_17275	GdRuS	3	-6.345	-6.84	0.000e+00	0.00225	0.554	0.726
tri_000_17299	NdSi ₂	3	-5.293	-5.754	-2.000e-06	0.00636	0.559	1.973
tri_000_17309	HClTb	3	-1.473	-4.334	0.000e+00	0.00547	0.928	1.983
tri_000_17352	MnRu	2	-8.742	-9.061	-1.000e-06	0.00315	0.267	0.23
tri_000_17371	DySb	2	-4.898	-5.227	3.000e-06	0.00294	0.797	0.691
tri_000_17390	CoCu	2	-5.042	-5.107	1.000e-06	0.00697	0.217	0.273
tri_000_17409	H ₂ GdMn	4	0.204	-4.884	1.000e-06	0.00773	0.687	0.714
tri_000_17414	CoMnP ₂	4	-6.708	-7.152	2.000e-06	0.00687	0.392	0.374
tri_000_17437	Tb ₂	2	-4.517	-4.548	-7.700e-06	0.00261	0.152	0.242
tri_000_17445	DyTb	2	-4.525	-4.535	5.200e-06	0.00089	0.079	0.046
tri_000_17450	CoOs	2	-8.739	-8.992	-1.300e-05	0.00418	0.142	0.093
tri_000_17457	AsGdGePt	4	-5.599	-5.737	2.000e-06	0.00722	0.322	0.359

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_17474	AlCo	2	-5.435	-5.71	6.000e-06	0.00782	0.339	0.185
tri_000_17480	ReRu	2	-10.808	-10.893	6.000e-06	0.00402	0.076	0.056
tri_000_17505	CSiTb	3	-6.136	-6.456	-3.000e-06	0.0027	0.756	0.505
tri_000_17517	CTb	2	-5.89	-6.822	-1.000e-06	0.00268	0.73	0.56
tri_000_17533	HBRu	3	-5.812	-6.344	-3.500e-05	0.00753	0.325	0.705
tri_000_17540	EuYb	2	-1.596	-1.644	-1.200e-06	0.00328	0.36	0.308
tri_000_17590	MnOsV	3	-9.532	-9.757	-1.000e-06	0.00689	0.459	0.377
tri_000_17595	FeGdSe	3	-5.653	-6.086	-1.000e-06	0.00896	0.736	0.935
tri_000_17622	GdTm	2	-4.513	-4.521	-6.000e-06	0.00094	0.084	0.05
tri_000_17629	FeLiO ₂	4	-6.358	-6.502	-2.000e-06	0.00516	0.288	0.25
tri_000_17650	PtRuSb	3	-5.701	-6.223	-1.300e-05	0.00242	0.235	0.209
tri_000_17652	AsRu	2	-6.503	-6.932	-2.000e-06	0.00374	0.403	0.501
tri_000_17700	DyPtSn	3	-5.322	-5.792	-1.000e-06	0.00411	1.024	1.022
tri_000_17710	FeLi	2	-4.604	-4.705	-1.730e-05	0.0031	0.178	0.088
tri_000_17721	AlCdNi	3	-3.158	-3.411	-1.800e-05	0.00456	0.635	0.45
tri_000_17759	MnPd	2	-6.582	-6.805	-4.000e-06	0.00244	0.364	0.225
tri_000_17767	DyEu	2	-3.029	-3.077	1.800e-06	0.00167	0.223	0.172
tri_000_17839	CoNdSi	3	-5.997	-6.263	-1.400e-05	0.00703	0.373	0.198
tri_000_17841	MnS ₂	3	-5.927	-6.062	-6.000e-06	0.00793	0.314	0.42
tri_000_17863	NaRuSe	3	-4.262	-4.697	-2.000e-06	0.00954	0.477	0.391
tri_000_17871	GdLu	2	-4.378	-4.509	6.400e-06	0.00531	0.294	0.201
tri_000_17901	CoCu	2	-5.079	-5.105	-1.600e-05	0.00648	0.113	0.101
tri_000_17921	NdSn	2	-4.725	-4.748	-3.100e-06	0.00506	0.154	0.188
tri_000_17925	FeNiRu	3	-7.315	-7.452	0.0000e+00	0.00582	0.192	0.146
tri_000_17926	CoNi	2	-6.034	-6.056	-2.000e-06	0.00258	0.066	0.086
tri_000_17930	MnNi	2	-7.034	-7.147	-4.000e-06	0.00447	0.182	0.143
tri_000_17943	HFeSi	3	-5.093	-5.746	0.0000e+00	0.00928	0.83	2.473
tri_000_17982	GdGeTi	3	-5.661	-5.788	1.000e-06	0.00822	0.348	0.326
tri_000_17986	AuRu	2	-5.677	-5.713	-3.000e-06	0.00631	0.136	0.128
tri_000_18006	DyNd	2	-4.541	-4.599	2.600e-06	0.00113	0.27	0.235
tri_000_18023	CoCuNi	3	-5.161	-5.252	-5.200e-05	0.00969	0.177	0.202
tri_000_18051	CoPtRu	3	-7.112	-7.326	-5.300e-05	0.00444	0.265	0.234
tri_000_18054	GaGdPt	3	-5.031	-5.552	-1.400e-05	0.00647	0.559	0.676
tri_000_18066	CoCu	2	-5.09	-5.112	0.0000e+00	0.00744	0.097	0.137
tri_000_18101	CoIr	2	-7.53	-7.846	-6.000e-06	0.00354	0.213	0.129
tri_000_18153	PtSbTb	3	-5.695	-5.985	-4.000e-06	0.00509	0.652	0.485
tri_000_18167	AuGaGd	3	-4.198	-4.374	-1.000e-06	0.00851	0.466	0.32
tri_000_18173	AlRu	2	-6.824	-6.962	0.0000e+00	0.00153	0.172	0.189
tri_000_18196	Si ₂ Yb	3	-4.373	-4.463	1.000e-06	0.0075	0.19	0.21
tri_000_18212	B ₂ Ru	3	-7.255	-7.606	-2.000e-06	0.00679	0.899	0.807
tri_000_18229	CDy	2	-5.377	-6.789	-3.000e-06	0.00369	1.154	1.431
tri_000_18249	FeRu	2	-8.123	-8.503	-3.000e-06	0.00688	0.468	0.529
tri_000_18261	CoMnSi ₂	4	-6.682	-6.977	-2.000e-06	0.00304	0.568	0.417
tri_000_18269	AcYb	2	-2.711	-2.73	3.000e-07	0.00259	0.158	0.107
tri_000_18285	DyZr	2	-6.362	-6.421	-2.000e-06	0.00827	0.217	0.207
tri_000_18299	TbY	2	-5.442	-5.497	-5.600e-05	0.00312	0.213	0.229
tri_000_18313	RhRu	2	-8.169	-8.226	-7.000e-06	0.00274	0.122	0.102
tri_000_18323	NbNi	2	-7.174	-7.763	-3.800e-05	0.00553	0.297	0.232
tri_000_18400	DyHg	2	23.745	-2.544	-2.100e-06	0.00294	0.931	1.3
tri_000_18412	AcNd	2	-4.213	-4.333	8.5000e-06	0.00315	0.287	0.081
tri_000_18429	RhRuV	3	-8.326	-8.618	-2.000e-06	0.00675	0.233	0.405
tri_000_18459	NdSi ₂	3	-5.712	-5.756	-2.000e-06	0.00582	0.18	0.135

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_18470	Pd ₂ SbTb	4	-5.227	-5.497	2.000e-06	0.00484	0.428	0.433
tri_000_18479	CdNNd	3	-4.937	-5.126	-5.000e-06	0.0082	0.225	0.356
tri_000_18482	NdTm	2	-4.514	-4.555	6.800e-06	0.00279	0.2	0.165
tri_000_18512	GaNi	2	-4.201	-4.476	3.300e-06	0.00797	0.391	0.436
tri_000_18548	MnTi	2	-8.29	-8.458	-1.900e-05	0.00049	0.23	0.163
tri_000_18561	AlMn	2	-6.249	-6.421	1.000e-06	0.00616	0.243	0.266
tri_000_18588	DyGePd	3	-5.272	-5.719	-1.000e-06	0.00248	0.577	0.433
tri_000_18639	NdPtTe	3	-5.612	-5.718	0.000e+00	0.00181	0.325	0.326
tri_000_18658	MnPd	2	-6.743	-6.825	-5.400e-05	0.00233	0.178	0.179
tri_000_18687	Be ₂ Dy	3	-3.877	-3.947	-8.000e-06	0.00137	0.271	0.194
tri_000_18688	DyPtSi	3	-5.733	-6.481	0.000e+00	0.00523	0.742	0.784
tri_000_18701	CoRu	2	-7.728	-7.967	-1.000e-06	0.00487	0.26	0.302
tri_000_18715	GdNd	2	-4.59	-4.63	1.500e-06	0.00103	0.189	0.13
tri_000_18718	NiSc	2	-5.771	-6.062	2.000e-06	0.00605	0.814	0.368
tri_000_18762	CsYb	2	-0.671	-0.881	5.000e-06	0.00322	0.741	0.934
tri_000_18766	S ₂ Tb	3	-5.002	-5.821	-1.000e-06	0.00274	2.35	2.347
tri_000_18768	GdGeSr	3	-3.094	-3.915	0.000e+00	0.00755	0.575	0.332
tri_000_18793	HfSbSeYb	4	-5.701	-5.796	-8.000e-06	0.00298	0.189	0.179
tri_000_18799	NdSi ₂	3	-5.527	-5.758	2.000e-06	0.00383	0.28	0.391
tri_000_18808	HBRu	3	-4.968	-6.161	0.000e+00	0.00468	0.32	1.508
tri_000_18809	DyNZn	3	-5.199	-5.399	-2.000e-06	0.00541	0.486	0.944
tri_000_18836	NbRu	2	-9.05	-9.769	3.000e-06	0.00292	0.228	0.169
tri_000_18856	LuTb	2	-4.439	-4.497	-2.800e-06	0.00539	0.194	0.244
tri_000_18862	LaNd	2	-4.739	-4.761	-4.400e-06	0.00213	0.163	0.11
tri_000_18868	BRuTb	3	-5.829	-7.229	-1.000e-06	0.00533	0.438	0.171
tri_000_18886	BeCo	2	-5.349	-5.545	-3.100e-05	0.00575	0.217	0.12
tri_000_18888	DyTh	2	-5.866	-5.934	-5.000e-06	0.00568	0.215	0.178
tri_000_18922	AlLaTb	3	-3.475	-4.528	-1.400e-05	0.0062	0.994	0.806
tri_000_18934	GdPb	2	-4.404	-4.421	7.600e-06	0.00272	0.131	0.092
tri_000_18946	HfRu	2	-9.599	-9.761	2.000e-06	0.00288	0.27	0.247
tri_000_18949	BaGdP	3	-3.308	-4.64	-1.600e-05	0.00488	0.596	0.405
tri_000_18962	CoTe ₂ Yb	4	-4.148	-4.337	-8.330e-04	0.00729	0.437	0.415
tri_000_18976	Ac ₂ Dy	3	-4.123	-4.158	0.000e+00	0.00885	0.132	0.181
tri_000_18984	NdRhTe	3	-5.188	-5.957	-1.000e-06	0.0036	0.982	2.465
tri_000_19009	NdSbSn	3	-4.264	-4.699	1.000e-06	0.00865	1.099	0.695
tri_000_19063	GdMgPt	3	-4.49	-4.824	0.000e+00	0.00182	1.086	2.182
tri_000_19076	GdSiTb	3	-4.249	-5.318	1.000e-06	0.00371	1.197	1.2
tri_000_19080	NiTaTb	3	-6.806	-6.993	0.000e+00	0.0068	0.829	0.363
tri_000_19081	NdYb	2	-3.019	-3.027	-4.500e-06	0.00181	0.12	0.116
tri_000_19113	Fe ₂ LiNd	4	-4.995	-5.504	-2.000e-05	0.00985	0.613	1.626
tri_000_19118	GdNaO	3	-5.245	-5.352	-4.000e-06	0.00824	0.229	0.268
tri_000_19128	RuV	2	-9.103	-9.164	0.000e+00	0.00688	0.404	0.273
tri_000_19132	CBeDy	3	-5.954	-6.095	-1.000e-06	0.00401	0.224	0.198
tri_000_19168	Be ₂ NdV	4	5.6	-4.719	0.000e+00	0.00438	0.827	1.728
tri_000_19177	GdNd	2	-4.621	-4.629	-6.400e-06	0.00125	0.1	0.1
tri_000_19210	MnPt	2	-7.185	-7.471	-3.000e-06	0.00358	0.334	0.291
tri_000_19219	Se ₂ Tb	3	-4.939	-5.247	-1.000e-06	0.00532	0.747	2.738
tri_000_19267	As ₂ Fe ₂	4	-5.766	-6.561	-3.000e-06	0.00351	0.487	0.293
tri_000_19274	BiGdPt	3	-5.394	-5.651	0.000e+00	0.00419	0.809	0.703
tri_000_19362	MnSiSn	3	4.836	-5.515	-1.000e-06	0.00995	0.855	0.608
tri_000_19389	HCuSeYb	4	-3.725	-3.909	1.000e-06	0.00705	0.374	0.408
tri_000_19392	BiGdNi	3	-4.592	-5.155	0.000e+00	0.00323	0.997	0.611

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_19474	CoPd	2	-5.589	-5.771	2.000e-06	0.00402	0.148	0.087
tri_000_19485	FeIr	2	-8.448	-8.519	-5.000e-06	0.00319	0.09	0.055
tri_000_19512	AuRu	2	-5.657	-5.714	-1.000e-06	0.00127	0.144	0.213
tri_000_19554	PrYb	2	-0.678	-2.973	-9.600e-06	0.00377	0.956	0.89
tri_000_19557	Co ₂ CrFe	4	-7.66	-7.791	-2.000e-06	0.00862	0.41	0.392
tri_000_19566	LuTb	2	-4.391	-4.499	-1.000e-07	0.00304	0.279	0.125
tri_000_19580	DyRu	2	-5.864	-6.73	-2.000e-06	0.00623	0.512	0.59
tri_000_19581	FePt	2	-6.605	-6.964	-1.000e-05	0.00738	0.231	0.154
tri_000_19592	DyNa	2	-2.593	-2.658	-3.500e-06	0.00494	0.303	0.273
tri_000_19607	GdMgTb	3	-3.393	-3.531	-7.000e-06	0.00292	0.506	0.424
tri_000_19609	DyOsSb	3	-6.391	-6.92	-1.000e-06	0.00582	1.161	1.0
tri_000_19680	GaYb	2	-2.285	-2.711	-1.200e-06	0.00285	0.876	0.803
tri_000_19691	BRuZr	3	-4.748	-8.58	-1.000e-06	0.00772	0.549	0.748
tri_000_19701	BMnP	3	-6.406	-7.048	0.000e+00	0.00462	0.829	0.877
tri_000_19710	AgRu	2	-4.751	-5.347	0.000e+00	0.00172	0.36	0.43
tri_000_19711	Cl ₂ Tb	3	-4.349	-4.682	-1.200e-05	0.00253	0.54	0.667
tri_000_19723	RuW	2	-10.456	-11.021	-5.000e-06	0.00723	0.159	0.401
tri_000_19740	AuNdSb	3	-4.534	-4.882	-1.000e-06	0.00209	0.821	2.521
tri_000_19766	BiSbYb	3	-3.134	-3.582	0.000e+00	0.00539	1.158	1.109
tri_000_19783	GdSb	2	-5.197	-5.292	-1.000e-06	0.00167	0.281	0.241
tri_000_19787	CGeTb	3	-5.893	-6.072	-9.000e-06	0.00738	0.502	0.455
tri_000_19788	GdTh	2	-5.942	-5.962	-3.000e-06	0.00716	0.113	0.127
tri_000_19791	DySSi	3	-4.954	-5.379	0.000e+00	0.00677	0.659	0.851
tri_000_19822	FeVZr	3	-7.74	-8.418	-1.000e-05	0.00882	0.907	0.493
tri_000_19824	MnRh	2	-8.064	-8.136	-1.000e-06	0.00054	0.131	0.135
tri_000_19836	MnZn	2	-4.426	-4.796	-1.800e-06	0.00336	0.342	0.117
tri_000_19847	CDyTe	3	-5.049	-5.632	-1.000e-06	0.00856	0.601	0.827
tri_000_19853	BaYb	2	-1.534	-1.614	1.470e-05	0.0009	0.361	0.395
tri_000_19867	AsGd	2	-5.698	-5.871	-8.000e-06	0.00516	0.238	0.154
tri_000_19873	NdTm	2	-4.543	-4.556	-1.210e-05	0.00228	0.117	0.087
tri_000_19886	FeMgZn	3	-3.019	-3.253	1.100e-06	0.00297	0.254	0.197
tri_000_19908	Cl ₂ Tb	3	-4.632	-4.694	-1.000e-06	0.00256	0.252	0.234
tri_000_19931	CoIr	2	-7.564	-7.846	1.000e-06	0.00196	0.207	0.172
tri_000_19942	B ₂ Ru	3	-7.161	-7.424	0.000e+00	0.00294	0.258	0.151
tri_000_19959	DyLu	2	-4.479	-4.485	-1.940e-05	0.00569	0.069	0.044
tri_000_19962	CuDyP	3	-5.488	-5.565	-1.200e-05	0.00825	0.187	0.219
tri_000_19996	DyTb	2	-4.529	-4.534	3.200e-06	0.0003	0.065	0.047
tri_000_20004	AlNbPdRu	4	-6.858	-7.218	-1.000e-05	0.00521	0.673	1.063
tri_000_20012	DyTm	2	-4.443	-4.497	-2.600e-06	0.00258	0.226	0.099
tri_000_20014	NaTb	2	-2.568	-2.685	-3.000e-07	0.00548	0.442	0.423
tri_000_20018	RuTm	2	-6.459	-6.831	-7.000e-06	0.00677	0.53	0.619
tri_000_20035	DyGe ₂	3	-4.747	-5.007	1.000e-06	0.00574	0.422	0.233
tri_000_20038	FeRu	2	-8.424	-8.608	-4.000e-06	0.00142	0.145	0.088
tri_000_20049	CuNi	2	-4.552	-4.573	-1.620e-05	0.00438	0.109	0.086
tri_000_20053	NdTb	2	-4.584	-4.614	-2.560e-05	0.00375	0.195	0.184
tri_000_20060	AuNdSn	3	-4.407	-4.716	-1.000e-06	0.00522	0.521	2.015
tri_000_20078	NiTm	2	-4.711	-5.328	0.000e+00	0.00464	1.086	0.537
tri_000_20122	Ru ₂	2	-8.42	-9.055	-3.000e-06	0.00986	0.455	0.206
tri_000_20125	AlDySi	3	-4.243	-4.983	1.000e-06	0.00573	1.002	0.652
tri_000_20147	CoSSe	3	-5.076	-5.169	-8.000e-06	0.00903	0.237	0.123
tri_000_20182	PrTb	2	-4.542	-4.618	6.900e-06	0.00246	0.317	0.495
tri_000_20215	AuSSeYb	4	-3.776	-4.046	-1.500e-05	0.00334	0.618	1.503

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_20216	Ga ₂ Tb	3	-3.712	-4.113	1.000e-06	0.00847	0.385	0.506
tri_000_20244	Dy ₂	2	-4.481	-4.528	-2.000e-07	0.00109	0.206	0.26
tri_000_20252	GeNdPd	3	-5.194	-5.716	-4.500e-05	0.0054	0.782	0.84
tri_000_20255	DyPr	2	-4.548	-4.601	-2.300e-06	0.0035	0.208	2.885
tri_000_20284	GdGePt	3	-5.882	-6.152	-2.500e-05	0.00853	0.519	0.398
tri_000_20297	AsRuSi	3	-6.156	-6.534	0.000e+00	0.00516	0.23	0.243
tri_000_20303	NiRe	2	-8.604	-8.876	5.000e-06	0.00971	0.367	0.48
tri_000_20314	GdNd	2	-4.621	-4.629	-1.700e-06	0.00413	0.085	0.084
tri_000_20346	Tb ₂	2	-4.541	-4.55	3.000e-06	0.00236	0.089	0.093
tri_000_20352	GdGeSi	3	-5.164	-5.364	-2.000e-06	0.00455	0.21	0.18
tri_000_20394	GdTe	2	-4.957	-5.176	-3.000e-06	0.00266	0.29	0.341
tri_000_20414	DyPdTb	3	-4.859	-5.167	2.000e-06	0.00504	0.488	0.519
tri_000_20428	NdPtSi	3	-6.144	-6.499	-2.500e-05	0.00506	0.244	0.323
tri_000_20459	MnZn	2	-4.725	-4.785	-2.000e-07	0.00474	0.19	0.19
tri_000_20533	PrYb	2	-2.997	-3.05	-6.000e-07	0.00456	0.269	0.181
tri_000_20563	FePt ₂	3	-6.297	-6.703	-6.000e-06	0.0074	0.278	0.331
tri_000_20565	MnNi	2	-7.043	-7.151	0.000e+00	0.00066	0.147	0.125
tri_000_20566	PtSeYb	3	-4.439	-4.881	-2.000e-06	0.00334	0.564	0.57
tri_000_20573	Al ₂ FeYb	4	-4.077	-4.378	4.000e-06	0.00243	0.205	0.361
tri_000_20587	GdTb	2	-4.548	-4.56	-1.200e-06	0.00185	0.09	0.071
tri_000_20595	NdRh ₂	3	-6.18	-6.407	-1.000e-05	0.00245	0.73	0.35
tri_000_20620	EuYb	2	-1.536	-1.64	-7.000e-07	0.00368	0.487	0.488
tri_000_20671	CaDyP	3	-4.415	-4.833	-1.000e-06	0.00394	0.672	0.681
tri_000_20766	B ₂ Ru	3	-7.361	-7.395	-2.000e-06	0.00817	0.114	0.132
tri_000_20796	NdTe ₂	3	-4.46	-4.722	-2.000e-06	0.00451	1.191	0.966
tri_000_20809	CuTbTe	3	-4.057	-4.487	-6.000e-06	0.00672	0.751	0.818
tri_000_20815	AlGdGe	3	-4.342	-4.917	-3.000e-06	0.00912	0.453	0.558
tri_000_20846	NdTb	2	-4.59	-4.614	2.780e-05	0.00152	0.185	0.166
tri_000_20855	FeOs	2	-9.501	-9.647	-1.000e-06	0.00217	0.159	0.084
tri_000_20861	OTb	2	-6.96	-7.404	-1.000e-06	0.00401	0.227	1.833
tri_000_20862	NdPSb	3	-4.379	-5.471	-5.000e-06	0.00565	1.55	1.04
tri_000_20868	HRuSb	3	-5.305	-5.414	9.000e-06	0.00965	0.557	0.446
tri_000_20896	BeFe	2	-5.795	-5.993	-2.000e-05	0.0048	0.209	0.142
tri_000_20923	GdTh	2	-5.865	-5.963	-2.000e-06	0.00614	0.308	0.299
tri_000_20924	Nd ₂	2	-4.654	-4.685	4.400e-06	0.0011	0.166	0.158
tri_000_20932	NaNd	2	-2.741	-2.815	-2.500e-06	0.0029	0.363	0.326
tri_000_20937	CAsDy	3	-5.656	-6.169	-2.000e-06	0.00526	0.521	1.74
tri_000_20940	AuGeYb	3	-3.481	-3.879	0.000e+00	0.00459	0.869	1.913
tri_000_20945	NiSn	2	-3.571	-4.587	-1.500e-06	0.00838	0.762	0.59
tri_000_20964	Ni ₂	2	-5.364	-5.386	-3.000e-06	0.00402	0.117	0.086
tri_000_20977	DyEuGa	3	-2.927	-3.359	-9.000e-06	0.00835	0.844	2.127
tri_000_20998	RuTh	2	-7.905	-8.425	-1.000e-06	0.00378	0.513	0.552
tri_000_21009	Si ₂ Yb	3	-4.413	-4.464	3.000e-06	0.00814	0.207	0.067
tri_000_21016	MnSn	2	-4.655	-5.895	-1.700e-05	0.00631	0.589	0.388
tri_000_21019	MnPtZr	3	-7.349	-7.936	1.000e-06	0.00376	0.795	0.567
tri_000_21028	NdSn	2	-4.723	-4.906	1.100e-06	0.00593	0.782	0.397
tri_000_21031	RuTb	2	-6.627	-6.869	0.000e+00	0.00841	0.681	0.686
tri_000_21033	AcNd	2	-4.255	-4.334	-4.800e-05	0.00512	0.195	0.096
tri_000_21035	Se ₂ Tb	3	-4.77	-5.258	-1.000e-06	0.00363	1.713	1.357
tri_000_21037	AuDy	2	-4.573	-4.657	-4.300e-06	0.00244	0.229	0.123
tri_000_21046	CdNdPd ₂	4	-3.852	-4.587	-3.100e-05	0.00652	0.629	0.311
tri_000_21060	MnTc	2	-9.373	-9.551	-5.000e-06	0.00665	0.218	0.258

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_21084	MnW	2	-9.581	-10.818	-7.000e-06	0.00648	1.153	1.793
tri_000_21109	B ₂ Ru	3	-7.116	-7.387	-2.000e-06	0.00738	0.217	0.127
tri_000_21110	TbY	2	-5.48	-5.494	-9.000e-06	0.00188	0.087	0.049
tri_000_21124	AlPrYb	3	-2.436	-3.407	-1.000e-06	0.00153	0.964	0.706
tri_000_21168	Se ₂ TbZr	4	-6.13	-6.414	0.000e+00	0.00309	0.469	0.604
tri_000_21193	B ₂ Ru	3	-7.388	-7.432	0.000e+00	0.00555	0.277	0.18
tri_000_21251	CoZn	2	-3.917	-3.981	-6.100e-06	0.00153	0.175	0.16
tri_000_21257	CdFeRu	3	-5.467	-5.684	-1.200e-05	0.00802	0.291	1.036
tri_000_21317	CoTc	2	-8.289	-8.602	-3.000e-05	0.00511	0.18	0.116
tri_000_21392	EuYb	2	-1.563	-1.64	-1.260e-05	0.00036	0.266	0.525
tri_000_21393	CrGdTe	3	-5.445	-5.576	1.500e-05	0.00559	0.112	0.191
tri_000_21401	AuRu	2	-5.436	-5.733	1.000e-06	0.00494	0.451	0.45
tri_000_21403	NiV	2	-7.109	-7.373	1.000e-06	0.00338	0.42	0.371
tri_000_21448	CRuSm	3	-5.85	-7.84	-1.000e-06	0.00395	0.66	0.9
tri_000_21461	NdRhTe	3	-5.27	-5.952	1.000e-06	0.00929	1.11	1.032
tri_000_21491	NdSb ₂	3	-4.033	-4.988	0.000e+00	0.00343	1.524	0.67
tri_000_21493	NdTb	2	-4.6	-4.614	-1.600e-06	0.00382	0.081	0.048
tri_000_21544	DyTm	2	-4.482	-4.498	7.000e-07	0.00239	0.09	0.13
tri_000_21546	RhSnTb	3	-5.605	-5.907	-6.000e-06	0.00691	0.801	0.806
tri_000_21552	FeVW	3	-9.58	-9.995	-1.000e-06	0.00502	0.462	0.293
tri_000_21556	NdSn	2	-4.682	-4.952	-4.100e-06	0.00442	0.798	0.726
tri_000_21560	TbTm	2	-4.397	-4.508	-9.600e-06	0.00237	0.318	0.364
tri_000_21637	PdSbYb	3	-4.075	-4.526	1.000e-06	0.00427	1.032	1.112
tri_000_21639	CuNdPtSe	4	-5.082	-5.175	1.000e-06	0.00854	0.373	1.372
tri_000_21669	IPtYb	3	-3.506	-3.748	-2.300e-05	0.00683	1.302	2.512
tri_000_21700	MgNd	2	3.209	-3.201	7.000e-07	0.0018	1.359	1.17
tri_000_21702	CoIr	2	-7.605	-7.843	-3.900e-05	0.00363	0.182	0.132
tri_000_21732	NiOs	2	-8.053	-8.194	-4.700e-05	0.00096	0.162	0.116
tri_000_21745	IrRu	2	-8.937	-9.085	6.000e-06	0.00822	0.17	0.12
tri_000_21752	CuFeW	3	-7.705	-7.962	-2.000e-06	0.00359	0.23	0.516
tri_000_21765	GaSiTb	3	-4.934	-4.937	-3.000e-06	0.00311	0.028	0.023
tri_000_21776	Au ₂ DySb	4	-3.929	-4.395	0.000e+00	0.00614	0.662	0.442
tri_000_21781	MnPd	2	-6.614	-6.823	-1.420e-04	0.0047	0.375	0.46
tri_000_21804	AsNNdRu	4	-6.379	-7.423	-2.000e-06	0.00784	0.266	0.676
tri_000_21816	GeRh ₂ Yb	4	-5.433	-5.545	0.000e+00	0.00229	0.393	0.326
tri_000_21893	FeSi	2	-6.912	-7.165	0.000e+00	0.00539	0.319	0.292
tri_000_21905	AcNaYb	3	-2.116	-2.194	-1.800e-06	0.00599	0.953	1.014
tri_000_21921	GaNdPd	3	-4.937	-5.078	-1.000e-06	0.00676	0.374	0.22
tri_000_21922	DyIn	2	-3.728	-3.827	-1.440e-05	0.00343	0.239	0.161
tri_000_21950	GeSbTb	3	-3.994	-4.766	5.000e-06	0.00753	1.113	0.908
tri_000_21994	NdSm	2	-4.635	-4.654	-3.700e-06	0.00289	0.153	0.198
tri_000_21995	AsYb	2	-0.803	-4.007	-8.000e-07	0.00046	1.495	2.596
tri_000_21999	GdOZn	3	-2.633	-5.109	-3.000e-06	0.00716	0.984	0.605
tri_000_22047	CrMnPd	3	-7.515	-7.718	-2.000e-06	0.00562	0.164	0.253
tri_000_22081	DyPtSe	3	-5.644	-5.822	-9.000e-06	0.00394	0.579	0.511
tri_000_22084	NbRu	2	-9.644	-9.696	0.000e+00	0.00396	0.226	0.355
tri_000_22100	CoSTb	3	-5.801	-6.328	-1.000e-06	0.00429	0.474	0.592
tri_000_22124	Se ₂ Tb	3	-4.838	-5.239	0.000e+00	0.00697	0.997	1.121
tri_000_22201	NbRu	2	-9.277	-9.774	-2.600e-05	0.00406	0.284	0.197
tri_000_22233	BNbRu	3	-7.831	-8.857	-1.000e-06	0.00229	0.886	1.674
tri_000_22251	GdP ₂	3	-5.285	-5.95	-3.000e-06	0.0046	0.601	1.654
tri_000_22289	AlAuFeMg	4	-3.749	-4.088	-4.000e-06	0.00327	0.378	2.573

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_22291	H ₂ Co	3	-4.131	-4.486	-1.000e-06	0.00389	0.433	0.901
tri_000_22331	DySm	2	-4.57	-4.573	-5.400e-06	0.00222	0.045	0.051
tri_000_22352	CAITb	3	-5.92	-6.068	0.000e+00	0.00298	0.267	0.307
tri_000_22365	CoDySi	3	-6.029	-6.293	-7.000e-06	0.00705	0.336	0.303
tri_000_22376	TbTe ₂	3	-4.556	-4.668	-1.000e-06	0.00619	0.763	0.514
tri_000_22385	DyLa	2	-4.625	-4.66	-2.100e-06	0.00183	0.165	0.104
tri_000_22404	NiSnTb	3	-4.779	-5.224	-2.000e-06	0.00697	0.835	1.79
tri_000_22437	B ₂ Ru	3	-7.061	-7.401	-1.000e-06	0.00297	0.233	0.114
tri_000_22466	PdSbTb	3	-5.374	-5.621	-2.000e-06	0.00769	0.358	0.498
tri_000_22474	NdSe ₂ Tm	4	-5.571	-5.696	-1.000e-06	0.00198	0.379	0.32
tri_000_22484	NiZn	2	-3.278	-3.427	-3.480e-05	0.00459	0.223	0.18
tri_000_22493	GdPr	2	-4.622	-4.634	1.100e-06	0.00249	0.13	0.082
tri_000_22516	TbTm	2	-4.488	-4.507	-1.000e-07	0.00133	0.109	0.164
tri_000_22519	GeLiOTb	4	0.873	-5.157	-7.000e-06	0.0084	1.078	1.148
tri_000_22531	DyTe	2	-4.996	-5.099	0.000e+00	0.00569	0.284	0.289
tri_000_22547	NdPtTe	3	-4.857	-5.685	-2.000e-06	0.00632	1.019	0.954
tri_000_22574	Eu ₂ PtTb	4	-3.636	-4.083	-1.000e-06	0.00742	0.547	0.588
tri_000_22578	GaSiTb	3	-4.84	-4.934	0.000e+00	0.0086	0.2	0.138
tri_000_22625	CdNi	2	-2.661	-2.901	-9.000e-07	0.00743	0.387	0.494
tri_000_22641	FeOs	2	-9.489	-9.647	-2.600e-05	0.00516	0.168	0.193
tri_000_22653	GdPPt	3	-6.679	-6.724	0.000e+00	0.0046	0.177	0.141
tri_000_22660	AlCo ₂ Fe	4	-6.298	-6.46	1.000e-06	0.00584	0.44	0.428
tri_000_22662	Si ₂ Tb	3	-5.648	-5.681	-3.000e-06	0.00209	0.212	0.145
tri_000_22665	DyMg	2	-2.905	-2.95	-3.300e-06	0.00289	0.275	0.276
tri_000_22677	B ₂ Ru	3	-7.272	-7.4	-1.000e-06	0.00463	0.18	0.179
tri_000_22697	RuZr	2	-8.756	-8.957	-8.000e-06	0.00489	0.261	0.136
tri_000_22716	DyPt ₂	3	-5.936	-6.494	-6.000e-06	0.00977	1.005	0.899
tri_000_22720	Dy ₂	2	-4.515	-4.525	8.000e-07	0.00429	0.076	0.051
tri_000_22733	CuNi	2	-4.53	-4.571	-3.600e-06	0.00614	0.083	0.107
tri_000_22755	DyY	2	-5.456	-5.483	-3.000e-06	0.00314	0.133	0.105
tri_000_22759	FeZn	2	-4.289	-4.405	1.000e-07	0.0054	0.294	0.161
tri_000_22760	FeNi	2	-6.537	-6.659	-1.000e-06	0.00312	0.202	0.176
tri_000_22762	SnYb	2	-3.057	-3.15	1.000e-07	0.00463	0.316	0.196
tri_000_22765	GaSnYb	3	-2.947	-3.231	4.000e-07	0.0079	0.658	0.54
tri_000_22771	CoOs ₂	3	-9.284	-9.637	-1.160e-04	0.00509	0.275	0.311
tri_000_22794	GePtYb	3	-4.922	-4.996	-1.000e-06	0.00557	0.381	0.408
tri_000_22814	CdNd	2	-2.772	-2.846	-1.800e-06	0.00107	0.474	0.372
tri_000_22883	CGdSb	3	-5.521	-5.892	-4.000e-06	0.0084	0.487	0.421
tri_000_22923	GaYb	2	-2.396	-2.425	-3.030e-05	0.00293	0.198	0.125
tri_000_22952	PdRu	2	-6.872	-6.981	-1.200e-05	0.00167	0.168	0.117
tri_000_22953	FePt	2	-6.807	-6.952	-7.000e-06	0.00305	0.225	0.193
tri_000_22976	CDy	2	-6.19	-6.84	-1.000e-06	0.00464	0.85	0.738
tri_000_22980	CdNi	2	-2.352	-2.899	-3.000e-07	0.00705	0.472	0.31
tri_000_22994	DySn	2	-4.628	-4.67	-6.200e-06	0.00394	0.151	0.093
tri_000_22997	DyTe	2	-4.608	-5.098	-2.000e-06	0.00481	0.61	0.766
tri_000_23020	IrMn	2	-8.839	-9.051	0.000e+00	0.00501	0.202	0.18
tri_000_23033	Br ₂ Dy	3	-3.855	-4.208	3.000e-06	0.00488	0.37	0.401
tri_000_23045	DySb	2	-5.206	-5.233	0.000e+00	0.00242	0.141	0.068
tri_000_23114	OsRu	2	-10.109	-10.255	-6.000e-06	0.00465	0.161	0.108
tri_000_23146	BrRhTb	3	-4.417	-5.144	1.000e-06	0.00632	0.625	0.803
tri_000_23158	PtSeYb	3	-4.305	-4.88	-1.000e-06	0.00438	0.851	0.727
tri_000_23168	DyEu	2	-2.965	-3.059	-6.000e-06	0.00103	0.614	0.344

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_23186	NdSeV	3	-5.527	-6.072	-1.000e-06	0.00401	1.233	0.821
tri_000_23191	RuZr	2	-8.915	-8.97	-1.200e-05	0.0045	0.173	0.114
tri_000_23213	GeMnNd	3	-5.967	-6.233	0.000e+00	0.0041	0.65	1.886
tri_000_23218	CCrNdSi	4	9.08	-7.076	0.000e+00	0.00994	0.927	1.375
tri_000_23268	MnV	2	-8.8	-9.133	-3.000e-06	0.00371	0.301	0.482
tri_000_23270	NdY	2	-5.452	-5.541	3.300e-05	0.0027	0.365	0.449
tri_000_23319	GdTm	2	-4.491	-4.521	3.000e-07	0.002	0.142	0.066
tri_000_23346	MnSn	2	-5.443	-5.803	0.000e+00	0.00658	0.529	0.276
tri_000_23416	AsCoDyGe	4	-5.64	-5.717	-1.000e-06	0.00327	0.359	0.27
tri_000_23456	CoRu	2	-7.836	-7.964	-3.000e-06	0.00141	0.145	0.146
tri_000_23462	AuNiOs	3	-5.996	-6.341	1.000e-06	0.00943	0.248	0.256
tri_000_23497	Cl ₂ Tb	3	-4.237	-4.676	-9.000e-06	0.00443	0.474	0.609
tri_000_23534	EuYb	2	-1.629	-1.642	-4.100e-06	0.00318	0.226	0.123
tri_000_23612	CoU	2	33.605	-8.796	-1.000e-06	0.00743	0.398	0.358
tri_000_23633	PSiTb	3	-3.676	-5.736	-4.000e-06	0.00246	0.773	1.647
tri_000_23656	AsCoTb	3	-5.754	-6.267	-2.000e-06	0.00249	0.612	0.679
tri_000_23698	CoPt ₂	3	-5.568	-6.305	-9.500e-05	0.00503	0.37	0.381
tri_000_23718	GeNdSi	3	-5.287	-5.428	-1.000e-06	0.00396	0.342	0.184
tri_000_23731	DyOsTe	3	-5.653	-6.578	-2.000e-06	0.00881	1.221	0.995
tri_000_23733	RuV	2	-9.088	-9.171	2.000e-06	0.00946	0.275	0.328
tri_000_23803	BDyIr	3	-4.105	-7.052	-9.000e-06	0.00529	0.715	0.537
tri_000_23843	FeW	2	-10.059	-10.296	-5.400e-05	0.00609	0.222	0.109
tri_000_23848	AlRuTi	3	-7.174	-7.298	1.000e-06	0.00446	0.097	0.333
tri_000_23882	GdPtTh	3	-6.525	-6.697	2.000e-06	0.005	0.46	0.64
tri_000_23883	B ₂ Ru	3	-7.287	-7.561	-1.000e-06	0.00853	0.75	0.354
tri_000_23888	FeRh	2	-7.456	-7.612	-1.000e-06	0.00326	0.244	0.282
tri_000_23892	FeNi	2	-6.612	-6.659	-1.300e-05	0.00326	0.134	0.137
tri_000_23914	CBNi	3	-6.058	-6.984	-9.000e-06	0.00587	0.541	0.567
tri_000_23953	CCaMn	3	-6.148	-6.481	-1.000e-05	0.00476	0.747	0.76
tri_000_23954	NdTm	2	-4.541	-4.556	-1.200e-06	0.00168	0.134	0.16
tri_000_23964	MnPt	2	-7.255	-7.472	1.000e-06	0.00298	0.288	0.259
tri_000_24039	CoRuV	3	-8.243	-8.333	5.000e-06	0.00868	0.223	0.261
tri_000_24041	Co ₄	4	-6.777	-6.822	-4.000e-06	0.00757	0.121	0.088
tri_000_24062	AlPYb	3	-4.003	-4.229	1.000e-06	0.00412	0.435	0.351
tri_000_24065	AgGeNaNd	4	-2.65	-3.516	-1.300e-05	0.00648	0.603	0.552
tri_000_24098	H ₂ Dy	3	-2.896	-4.418	-4.000e-06	0.00282	0.484	0.726
tri_000_24111	FePt	2	-6.917	-6.952	-4.000e-06	0.00319	0.077	0.099
tri_000_24122	FeRe	2	-10.107	-10.249	-1.300e-05	0.00671	0.156	0.127
tri_000_24124	NdPtTe	3	-5.183	-5.711	-3.000e-06	0.00561	0.969	0.762
tri_000_24149	GdSi ₂	3	-5.559	-5.7	-2.000e-06	0.00413	0.279	0.27
tri_000_24197	B ₂ Ru	3	-7.127	-7.544	-1.000e-06	0.00574	0.71	0.702
tri_000_24220	DySTi	3	-6.434	-6.48	5.000e-06	0.00238	0.114	0.177
tri_000_24222	NiPt	2	-5.233	-5.748	-8.000e-06	0.004	0.299	0.335
tri_000_24242	Ac ₂ Dy	3	-3.966	-4.157	-3.000e-06	0.00745	0.345	0.214
tri_000_24262	RuSe ₂	3	-4.928	-5.534	-3.000e-06	0.00491	0.514	0.451
tri_000_24297	NiZn	2	-3.324	-3.428	-2.000e-06	0.00148	0.146	0.14
tri_000_24301	GdYb	2	-2.895	-2.931	-7.100e-06	0.00234	0.23	0.272
tri_000_24337	MnS ₂ Sb	4	-4.993	-5.467	1.800e-05	0.00866	0.519	1.493
tri_000_24350	Ni ₂	2	-5.378	-5.386	-1.000e-06	0.00596	0.062	0.058
tri_000_24368	FeRu	2	-8.263	-8.61	0.000e+00	0.00665	0.291	0.355
tri_000_24421	B ₂ Ru	3	-7.289	-7.399	-1.000e-06	0.00935	0.138	0.102
tri_000_24494	MnTc	2	-9.27	-9.556	-3.000e-06	0.00689	0.104	0.367

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_24500	GdMgSb	3	-2.148	-3.82	-2.000e-06	0.00376	1.174	1.36
tri_000_24534	AlMn	2	-6.283	-6.423	3.000e-06	0.00074	0.223	0.151
tri_000_24571	GdIrTe	3	-5.924	-6.332	0.000e+00	0.00721	0.784	0.65
tri_000_24593	NdRb	2	-2.228	-2.303	0.000e+00	0.0013	0.341	0.284
tri_000_24597	AlNd	2	-4.234	-4.272	9.000e-07	0.00812	0.167	0.12
tri_000_24611	BaSiTb	3	-2.485	-4.186	1.000e-06	0.00164	0.87	0.536
tri_000_24623	GeNdSb	3	-4.118	-4.884	-6.000e-06	0.00457	0.944	0.614
tri_000_24625	SiTb	2	-4.598	-5.466	1.000e-06	0.00176	0.905	0.604
tri_000_24640	CoGdP	3	-6.363	-6.71	-3.300e-05	0.00873	0.41	0.522
tri_000_24654	AlGdSi	3	-5.022	-5.218	-1.000e-06	0.0053	0.334	0.225
tri_000_24665	NdPtSb	3	-5.555	-6.071	-1.000e-06	0.00441	0.814	1.019
tri_000_24678	Br ₂ Mn	3	-3.357	-4.16	-1.000e-06	0.00673	0.641	0.515
tri_000_24689	AsGdSi	3	-4.965	-5.461	1.000e-06	0.00248	0.505	0.545
tri_000_24691	DyPSi	3	-5.157	-5.739	-2.000e-06	0.00135	1.14	1.156
tri_000_24700	RuS ₂	3	-5.778	-5.985	-3.000e-06	0.00206	0.72	0.712
tri_000_24777	GdS ₂ Ta	4	-7.24	-7.365	0.000e+00	0.00526	0.373	1.199
tri_000_24843	PdSbYb	3	-4.012	-4.542	-3.000e-06	0.00571	0.972	1.901
tri_000_24846	BrDyLiTe	4	-3.658	-4.04	0.000e+00	0.00835	0.53	0.439
tri_000_24858	DyGd	2	-4.533	-4.552	-2.100e-06	0.00233	0.124	0.113
tri_000_24880	CoNdSn	3	-5.15	-5.523	-2.000e-06	0.00843	0.653	0.481
tri_000_24913	NbRu	2	-9.454	-9.684	-2.000e-06	0.00482	0.133	0.144
tri_000_24914	GdYb	2	-2.82	-2.928	-5.700e-06	0.00266	0.406	0.442
tri_000_24920	CDyTb	3	-6.266	-6.363	-1.000e-06	0.00256	0.223	0.35
tri_000_24926	GdYb	2	-2.858	-2.931	8.600e-06	0.00709	0.309	0.144
tri_000_24973	RuTb	2	-6.573	-6.841	-6.000e-06	0.00231	0.521	0.469
tri_000_24980	AlNi	2	-4.862	-5.076	1.000e-06	0.00678	0.229	0.125
tri_000_25005	FeIr	2	-8.328	-8.512	-3.000e-06	0.00375	0.172	0.116
tri_000_25020	As ₂ Ni ₂	4	-0.123	-5.141	0.000e+00	0.00981	0.768	0.412
tri_000_25021	GdPr	2	-1.574	-4.592	-3.000e-07	0.00227	0.985	0.816
tri_000_25060	GaGdTh	3	-4.554	-5.088	-5.000e-06	0.00612	0.527	0.316
tri_000_25088	Si ₂ Yb	3	-4.398	-4.464	0.000e+00	0.00356	0.265	0.08
tri_000_25113	LaNd	2	-4.745	-4.761	-5.200e-06	0.00291	0.123	0.152
tri_000_25129	NdTb	2	-4.584	-4.609	1.200e-06	0.00442	0.152	0.151
tri_000_25135	GdTe	2	-4.664	-5.171	-2.000e-06	0.00468	0.569	0.706
tri_000_25136	GeSiTb	3	-5.122	-5.323	-7.000e-06	0.00569	0.372	0.215
tri_000_25148	GaNdSb	3	-4.349	-4.513	-6.000e-06	0.00659	0.54	0.5
tri_000_25162	CoDyTe	3	-4.954	-5.577	-2.000e-06	0.0098	1.117	0.959
tri_000_25164	NdPr	2	-4.66	-4.693	-8.300e-06	0.00169	0.186	0.129
tri_000_25168	Nd ₂	2	-4.662	-4.685	-1.500e-06	0.00592	0.174	0.165
tri_000_25174	Be ₃ Dy	4	2.563	-3.853	0.000e+00	0.00232	1.78	1.9
tri_000_25206	Ge ₂ Mn	3	-4.964	-5.859	-1.000e-06	0.00708	0.614	0.616
tri_000_25243	NdSi	2	-5.22	-5.49	-1.000e-06	0.00145	0.755	0.362
tri_000_25298	FePd	2	-6.281	-6.333	-1.900e-05	0.00155	0.152	0.18
tri_000_25302	NdSe ₂	3	-4.918	-5.356	-1.000e-05	0.00502	1.857	1.874
tri_000_25320	TeYb	2	-3.162	-3.687	-3.000e-07	0.00582	0.401	0.289
tri_000_25321	ReRu	2	-10.56	-10.896	-5.000e-06	0.00348	0.221	0.207
tri_000_25333	GeNdPt	3	-5.996	-6.149	-1.000e-05	0.0079	0.27	0.443
tri_000_25361	B ₂ Ru	3	-7.292	-7.399	-7.000e-06	0.00255	0.141	0.1
tri_000_25363	CaGd	2	-3.082	-3.147	2.000e-07	0.00265	0.268	0.09
tri_000_25379	NdYb	2	-3.022	-3.028	-3.820e-05	0.00273	0.065	0.047
tri_000_25394	BBeRu	3	-6.437	-6.71	-3.000e-06	0.00519	0.387	0.281
tri_000_25395	FeRe	2	-10.052	-10.244	2.000e-06	0.00874	0.178	0.196

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_25408	HfMn ₂ Os	4	-9.017	-9.55	-1.000e-06	0.00715	0.331	0.808
tri_000_25433	AgAuNd	3	-3.842	-4.097	0.000e+00	0.00383	0.77	1.92
tri_000_25438	PrYb	2	-2.997	-3.049	-6.000e-07	0.00482	0.269	0.239
tri_000_25467	AlMgMn	3	-4.214	-4.503	0.000e+00	0.00436	0.527	0.796
tri_000_25482	IrRu	2	-8.212	-9.009	-1.000e-05	0.0019	0.517	0.242
tri_000_25534	NdTm	2	-4.523	-4.558	-5.600e-06	0.00447	0.194	0.152
tri_000_25544	CrNdSb ₂	4	-5.599	-5.81	9.000e-06	0.00427	0.251	0.17
tri_000_25557	AcYb	2	-2.604	-2.73	4.000e-07	0.0021	0.346	0.348
tri_000_25623	FeRu	2	-8.496	-8.61	-3.000e-06	0.00244	0.17	0.105
tri_000_25647	In ₂ Ru	3	-4.383	-4.584	-2.000e-06	0.00911	0.235	0.247
tri_000_25675	DyPtTe	3	-5.233	-5.586	-9.000e-06	0.00871	0.678	0.623
tri_000_25684	DyGeRu	3	-6.221	-6.609	-5.000e-06	0.00786	0.923	2.129
tri_000_25693	GdYb	2	-2.865	-2.925	2.300e-06	0.00364	0.286	0.189
tri_000_25699	LaNd	2	-4.751	-4.761	5.100e-06	0.00114	0.115	0.053
tri_000_25717	NdSbSr	3	-1.808	-3.963	-1.000e-06	0.0041	0.834	0.432
tri_000_25722	NiTi	2	-6.582	-6.736	0.000e+00	0.00409	0.239	0.192
tri_000_25739	GdSn	2	-4.67	-4.704	5.000e-07	0.00491	0.165	0.192
tri_000_25743	CBeRu	3	-6.674	-7.136	-2.000e-06	0.00239	0.795	1.41
tri_000_25839	Pt ₂ SnYb	4	-4.83	-5.15	-1.000e-06	0.00523	0.432	0.264
tri_000_25862	CuNi	2	-4.513	-4.575	-2.500e-06	0.00394	0.201	0.202
tri_000_25887	GeNi	2	-4.514	-5.089	1.000e-06	0.00241	0.401	0.303
tri_000_25892	AsDyNi	3	-5.311	-5.946	-2.100e-05	0.0099	0.711	0.855
tri_000_25903	CoNi	2	-5.999	-6.057	2.000e-06	0.00898	0.173	0.268
tri_000_25947	DyTb	2	-4.499	-4.536	-3.000e-07	0.00122	0.171	0.159
tri_000_25949	NdSe ₂	3	-4.275	-5.361	-1.000e-06	0.00599	1.523	2.285
tri_000_25976	EuYb	2	-1.574	-1.643	-5.200e-06	0.00202	0.347	0.434
tri_000_25987	DyS ₂	3	-5.193	-5.806	0.000e+00	0.0043	1.61	1.787
tri_000_26003	GeNdS	3	-4.549	-5.307	0.000e+00	0.00364	0.846	1.576
tri_000_26070	NdSe ₂	3	-5.044	-5.372	-1.000e-06	0.00261	1.673	1.467
tri_000_26110	DySm	2	-4.524	-4.572	2.400e-06	0.00152	0.167	0.153
tri_000_26117	PdRu	2	-6.954	-6.985	-7.000e-06	0.00219	0.113	0.112
tri_000_26154	DyPr	2	-4.581	-4.597	2.000e-07	0.00307	0.158	0.151
tri_000_26183	DySe ₂	3	-4.3	-5.226	0.000e+00	0.00254	1.029	0.95
tri_000_26189	SnTb	2	-4.426	-4.688	-7.000e-07	0.00377	0.45	0.445
tri_000_26191	GdSi ₂	3	-5.678	-5.702	-9.000e-06	0.00146	0.188	0.104
tri_000_26201	Tb ₂	2	-4.531	-4.549	-3.400e-06	0.00356	0.137	0.136
tri_000_26250	FeV	2	-8.46	-8.552	2.000e-06	0.00407	0.287	0.315
tri_000_26299	FeLu	2	-5.731	-5.869	-1.500e-05	0.00496	0.291	0.395
tri_000_26311	RuSi	2	-7.457	-7.796	0.000e+00	0.00095	0.241	0.158
tri_000_26329	PtSnTb	3	-5.45	-5.762	-3.000e-06	0.00869	1.257	1.074
tri_000_26334	FeW	2	-10.041	-10.295	0.000e+00	0.00659	0.214	0.192
tri_000_26345	HgTb	2	-2.635	-2.683	-6.700e-06	0.00212	0.185	0.212
tri_000_26356	HfRu	2	-9.336	-9.851	-1.300e-05	0.00283	0.177	0.139
tri_000_26400	GdSbSi	3	-4.305	-5.113	1.000e-06	0.0054	0.629	0.485
tri_000_26406	H ₂ Mn	3	-4.039	-5.13	-6.000e-06	0.0045	0.285	0.577
tri_000_26444	GdTm	2	-4.478	-4.52	7.000e-07	0.00447	0.187	0.196
tri_000_26460	SiSrYb	3	-2.318	-2.996	4.600e-06	0.00119	0.695	0.586
tri_000_26467	MnOs	2	-9.583	-10.104	-2.000e-06	0.00178	0.345	0.342
tri_000_26469	RuZr	2	-8.822	-8.964	-1.000e-06	0.00313	0.391	0.322
tri_000_26474	CuDyP	3	-5.553	-5.564	0.000e+00	0.0015	0.073	0.113
tri_000_26478	DyPdSn	3	-5.153	-5.416	1.000e-06	0.00735	0.513	0.688
tri_000_26481	Nd ₂	2	-4.677	-4.685	-1.000e-07	0.00206	0.073	0.045

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_26489	NdTm	2	-4.55	-4.559	-1.420e-05	0.00507	0.061	0.052
tri_000_26506	LiSTb	3	-4.511	-4.574	-2.000e-06	0.00524	0.174	0.259
tri_000_26509	CoGe ₂ Tb	4	-5.463	-5.554	2.000e-06	0.00669	0.373	1.222
tri_000_26523	IrNi	2	-6.667	-7.105	7.000e-06	0.00469	0.217	0.137
tri_000_26531	PtTbTe	3	-5.183	-5.609	-1.000e-06	0.00276	0.884	0.717
tri_000_26532	GdSeZn	3	-3.466	-3.904	-1.000e-06	0.00331	0.627	0.679
tri_000_26568	FeP ₂ Ru	4	-6.341	-7.297	4.000e-06	0.0067	0.438	1.061
tri_000_26575	GdPr	2	-4.595	-4.628	-9.000e-07	0.00419	0.138	0.089
tri_000_26577	CdNdSe ₂	4	-4.173	-4.263	2.000e-06	0.00658	0.362	0.23
tri_000_26579	DyEu	2	-3.034	-3.077	-1.760e-05	0.00283	0.191	0.116
tri_000_26629	H ₃ Mn	4	-4.237	-4.537	-2.000e-06	0.00612	0.092	1.589
tri_000_26646	GdS ₂ Ta	4	-7.119	-7.365	-1.000e-06	0.00619	0.574	0.466
tri_000_26677	PdTb ₂	3	-5.004	-5.189	-1.000e-06	0.00436	0.462	0.421
tri_000_26693	Ge ₂ Tb	3	-4.532	-5.039	-1.000e-06	0.00806	0.636	0.683
tri_000_26720	CuGdO	3	-5.475	-5.556	-4.000e-06	0.00824	0.181	0.123
tri_000_26822	CoPt	2	-5.954	-6.402	1.000e-06	0.00287	0.389	0.344
tri_000_26859	DySe ₂	3	-4.634	-5.241	-2.000e-06	0.00427	0.538	0.57
tri_000_26861	B ₂ Ru	3	-7.353	-7.429	0.000e+00	0.00537	0.404	0.12
tri_000_26864	GdGe	2	-4.67	-5.248	0.000e+00	0.00267	0.609	0.357
tri_000_26878	AuTeYb	3	-3.216	-3.46	-2.000e-06	0.00346	0.815	0.798
tri_000_26964	CGdTe	3	-5.038	-5.597	0.000e+00	0.00758	0.664	0.618
tri_000_27011	GaGdSr	3	-2.469	-3.155	-4.300e-06	0.00641	1.074	0.841
tri_000_27018	BeMn	2	-6.076	-6.33	0.000e+00	0.00063	0.266	0.139
tri_000_27062	MgPtTb	3	-4.54	-4.825	-2.000e-06	0.00197	0.887	0.576
tri_000_27074	CaNd	2	-3.238	-3.245	5.000e-07	0.00175	0.081	0.07
tri_000_27077	FeRh	2	-7.226	-7.569	-5.000e-06	0.00194	0.49	0.3
tri_000_27118	AlGdN	3	-5.622	-6.222	0.000e+00	0.00497	0.799	0.417
tri_000_27180	DySn	2	-4.644	-4.665	2.900e-06	0.00416	0.106	0.15
tri_000_27185	MnSn	2	-5.105	-5.791	-1.200e-05	0.00891	0.712	0.632
tri_000_27197	LiNiV	3	-5.137	-5.343	0.000e+00	0.0045	0.275	0.48
tri_000_27202	CGdTe	3	-5.096	-5.597	-2.000e-06	0.00554	1.042	1.147
tri_000_27209	NiV	2	-7.135	-7.399	2.000e-06	0.00576	0.477	0.29
tri_000_27213	AuTbTe	3	-3.933	-4.566	-1.000e-06	0.00379	0.638	0.516
tri_000_27230	AlNi	2	-5.057	-5.078	-1.000e-06	0.00644	0.104	0.096
tri_000_27237	GeNdZn	3	-3.969	-4.128	-2.000e-06	0.00693	0.283	0.153
tri_000_27276	RuZr	2	-8.912	-8.971	2.000e-06	0.00661	0.166	0.121
tri_000_27279	DyGd	2	-4.541	-4.552	-8.200e-06	0.00132	0.071	0.038
tri_000_27315	TbTl	2	-3.575	-3.609	-1.360e-05	0.00307	0.149	0.031
tri_000_27352	FeOs	2	-9.344	-9.645	0.000e+00	0.00243	0.253	0.295
tri_000_27397	FePt	2	-6.891	-6.945	-2.000e-05	0.00228	0.143	0.185
tri_000_27399	PdSbTb	3	-5.345	-5.628	-3.000e-06	0.00359	0.522	0.665
tri_000_27412	GdPt ₃	4	-5.897	-6.159	0.000e+00	0.00637	0.865	1.756
tri_000_27460	BGdP	3	-6.072	-6.126	-1.000e-06	0.0028	0.161	0.119
tri_000_27465	NdSc	2	-5.354	-5.381	0.000e+00	0.00057	0.189	0.081
tri_000_27467	BRuY	3	-7.001	-7.869	0.000e+00	0.00796	0.361	0.253
tri_000_27469	LaTb	2	-4.652	-4.678	-1.200e-06	0.00503	0.208	0.144
tri_000_27473	NdSe ₂	3	-5.041	-5.369	-2.000e-06	0.0047	1.501	2.022
tri_000_27507	PbYb	2	-2.805	-2.96	3.000e-07	0.00336	0.422	0.53
tri_000_27557	TbZr	2	-0.776	-6.202	0.000e+00	0.00387	1.023	0.957
tri_000_27572	NiOs	2	-8.141	-8.209	-8.000e-06	0.00451	0.132	0.066
tri_000_27610	FeZn	2	-3.779	-4.416	-2.300e-06	0.00358	0.721	1.113
tri_000_27616	DyPtSe	3	-5.203	-5.796	-2.000e-06	0.00545	1.092	0.751

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_27650	MnSm	2	-4.704	-5.899	-1.000e-06	0.00179	0.457	0.32
tri_000_27663	NaYb	2	-1.261	-1.313	2.000e-07	0.00292	0.351	0.516
tri_000_27666	S ₂ SnTb	4	-4.303	-5.313	-1.000e-06	0.00251	1.052	1.097
tri_000_27669	HfRu	2	-9.735	-9.769	-6.000e-06	0.00407	0.166	0.064
tri_000_27714	FeOs	2	-9.567	-9.652	-5.600e-05	0.00591	0.127	0.14
tri_000_27726	DyNi	2	-4.65	-5.153	-2.000e-05	0.00186	0.844	0.336
tri_000_27731	MnRu	2	-9.0	-9.07	-2.000e-06	0.00697	0.122	0.147
tri_000_27758	AgGdP	3	-4.921	-4.983	3.000e-06	0.00498	0.198	0.204
tri_000_27806	GdTh	2	-5.93	-5.962	-1.400e-05	0.00478	0.198	0.148
tri_000_27834	Nd ₂	2	-4.676	-4.685	5.000e-07	0.00088	0.089	0.06
tri_000_27840	NdNiSi	3	-5.901	-5.912	-1.650e-04	0.00666	0.058	0.042
tri_000_27864	GdPdSe	3	-4.961	-5.57	-1.700e-05	0.00794	0.958	0.898
tri_000_27902	MnRh	2	-7.651	-8.032	0.000e+00	0.00173	0.433	0.207
tri_000_27910	GdSbTi	3	-5.341	-5.685	-3.900e-05	0.00993	0.472	0.613
tri_000_27912	NiRe	2	-8.847	-8.878	3.000e-06	0.00218	0.107	0.124
tri_000_27934	AlPdYb	3	-4.104	-4.134	0.000e+00	0.00195	0.23	0.159
tri_000_27935	NdNiSbZn	4	-4.004	-4.353	-1.000e-06	0.00832	0.669	0.617
tri_000_27948	GdTb	2	-4.531	-4.563	-7.000e-07	0.00065	0.173	0.183
tri_000_27957	GdNdSi	3	-3.935	-5.205	-2.000e-06	0.00267	0.578	0.52
tri_000_28000	NiSc	2	-5.704	-6.045	-2.800e-05	0.00201	0.671	0.587
tri_000_28024	RuTm	2	-5.692	-6.765	-4.000e-06	0.00336	0.316	0.193
tri_000_28055	NiSeTb	3	-5.233	-5.566	0.000e+00	0.00997	0.454	1.96
tri_000_28071	AlPdYb	3	-3.879	-4.136	1.000e-06	0.00387	0.177	0.448
tri_000_28095	GeSnYb	3	-3.653	-3.781	1.000e-06	0.00539	0.175	0.248
tri_000_28116	CNdSe	3	-5.201	-5.907	-1.000e-06	0.00413	0.619	0.652
tri_000_28132	CDyZr	3	-7.679	-7.819	-1.000e-06	0.00735	0.231	0.135
tri_000_28220	SeTbTe	3	-4.788	-4.899	0.000e+00	0.00526	0.342	0.322
tri_000_28239	CoTe ₂	3	-4.393	-4.632	0.000e+00	0.00489	0.441	0.281
tri_000_28249	CoFe	2	-7.321	-7.488	-2.000e-05	0.00415	0.203	0.228
tri_000_28267	AuMnRh	3	-5.999	-6.265	-1.000e-06	0.00988	0.292	0.355
tri_000_28274	NdSiSr	3	-3.215	-4.061	1.000e-06	0.00486	0.558	0.315
tri_000_28275	GdY	2	-5.391	-5.506	0.000e+00	0.00466	0.294	0.171
tri_000_28280	EuYb	2	-1.605	-1.641	-5.000e-05	0.00179	0.203	0.24
tri_000_28301	NdRh ₂ Sb	4	-5.95	-6.292	0.000e+00	0.00303	0.481	0.405
tri_000_28318	GdLu	2	-4.481	-4.505	7.600e-06	0.00219	0.124	0.141
tri_000_28323	OsRu	2	-9.9	-10.24	3.000e-06	0.00263	0.179	0.254
tri_000_28329	GdTe	2	-5.059	-5.176	-6.000e-06	0.00258	0.286	0.309
tri_000_28337	CDyMn	3	-7.284	-7.666	-4.000e-06	0.00564	0.701	0.718
tri_000_28341	FeZn	2	-4.357	-4.411	-1.360e-05	0.00313	0.177	0.126
tri_000_28346	GdPtS	3	-5.474	-6.119	7.000e-06	0.0023	1.09	1.066
tri_000_28347	Si ₂ Yb	3	-4.404	-4.463	0.000e+00	0.0028	0.166	0.153
tri_000_28365	CBeRu	3	-6.628	-7.209	0.000e+00	0.00384	0.539	0.497
tri_000_28383	CoGaIr	3	-5.721	-6.289	-5.000e-06	0.00267	0.245	0.116
tri_000_28391	GdRhTe	3	-5.089	-5.872	-3.000e-06	0.0053	0.944	0.846
tri_000_28406	RhSiTb	3	-6.515	-6.676	-3.100e-05	0.00628	0.221	0.1
tri_000_28432	HMnRu	3	-7.156	-7.197	0.000e+00	0.00508	0.079	0.083
tri_000_28438	FeRu	2	-8.389	-8.609	3.000e-06	0.00073	0.243	0.24
tri_000_28466	AuDyGe	3	-4.526	-4.877	-4.100e-05	0.0059	0.462	0.308
tri_000_28515	IrRu	2	-8.845	-9.075	-6.000e-06	0.00402	0.227	0.197
tri_000_28565	DyZr	2	-6.375	-6.422	-1.100e-05	0.0042	0.174	0.099
tri_000_28619	LuTb	2	-4.425	-4.498	1.200e-06	0.00378	0.23	0.161
tri_000_28626	NdNiTe	3	-5.026	-5.343	-1.000e-06	0.0072	0.558	0.489

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_28682	MnOs	2	-9.943	-10.108	-1.000e-06	0.00251	0.176	0.126
tri_000_28707	AlCo	2	-5.31	-5.706	-2.600e-05	0.00749	0.426	0.34
tri_000_28710	CMnY	3	-7.922	-8.293	3.000e-06	0.0074	0.525	0.417
tri_000_28713	NdTb	2	-4.588	-4.614	-5.300e-06	0.00111	0.172	0.171
tri_000_28724	DyLa	2	-4.598	-4.66	8.000e-07	0.0013	0.297	0.28
tri_000_28743	AsSrYb	3	-2.034	-3.309	-8.100e-06	0.00497	0.773	0.517
tri_000_28766	BeMn	2	-6.01	-6.331	-2.000e-06	0.00731	0.241	0.135
tri_000_28787	CoPt	2	-5.779	-6.399	-1.100e-05	0.00675	0.541	0.515
tri_000_28804	CoIr	2	-7.366	-7.847	3.000e-06	0.00473	0.211	0.24
tri_000_28850	DyPTi	3	-6.442	-6.653	0.000e+00	0.00253	0.367	0.485
tri_000_28873	DyGeOs	3	-6.978	-7.144	-1.500e-05	0.00714	0.472	0.286
tri_000_28898	NdOTe	3	-5.788	-6.326	-1.100e-05	0.00931	0.33	0.485
tri_000_28919	DyS ₂	3	-5.348	-5.799	0.000e+00	0.00381	1.584	1.345
tri_000_28934	CoV	2	-7.792	-8.102	1.700e-05	0.00873	0.78	0.719
tri_000_28952	Nd ₂ Pt ₂	4	-5.993	-6.482	-2.000e-06	0.00236	0.474	0.321
tri_000_28990	GdSiTe	3	-3.969	-4.866	-2.000e-06	0.0029	1.548	1.199
tri_000_28994	CNbRu	3	-9.36	-9.626	-1.000e-06	0.00223	0.219	0.195
tri_000_29004	DyPtTe	3	-4.883	-5.569	0.000e+00	0.0076	0.928	0.826
tri_000_29010	GaTb	2	-3.809	-4.048	4.900e-06	0.0044	0.532	0.281
tri_000_29033	SbTb	2	-4.967	-5.258	-2.000e-06	0.00443	0.759	0.66
tri_000_29041	HGdSSi	4	-4.299	-4.813	-1.000e-06	0.0031	0.371	1.191
tri_000_29046	GdPtSi	3	-6.495	-6.509	0.000e+00	0.00395	0.148	0.172
tri_000_29071	RuZr	2	-8.454	-8.915	-2.000e-06	0.00499	0.396	0.304
tri_000_29080	DyZr	2	-6.383	-6.422	-1.000e-06	0.00533	0.154	0.117
tri_000_29107	Be ₂ GdRu	4	5.133	-5.209	0.000e+00	0.00275	0.587	1.744
tri_000_29112	NdRhY	3	-6.468	-6.572	0.000e+00	0.00122	0.305	0.475
tri_000_29124	MnTm	2	-5.721	-6.051	7.000e-06	0.00314	0.446	0.392
tri_000_29131	DyNiTe	3	-4.77	-5.226	0.000e+00	0.0061	0.771	0.618
tri_000_29161	MnZn	2	-4.619	-4.796	-2.400e-06	0.00146	0.261	0.079
tri_000_29165	CoTb	2	-4.331	-5.623	0.000e+00	0.00403	1.003	0.891
tri_000_29176	CdYb	2	-1.288	-1.329	-5.200e-06	0.00282	0.356	0.273
tri_000_29196	B ₂ Ru	3	-7.373	-7.395	0.000e+00	0.00847	0.072	0.046
tri_000_29199	GdSTi	3	-6.407	-6.477	-1.000e-06	0.00349	0.148	0.196
tri_000_29211	NiV ₂	3	-7.693	-7.941	-2.000e-06	0.00666	0.491	0.257
tri_000_29225	GeSbYb	3	-3.424	-3.791	-1.000e-06	0.00803	0.797	0.481
tri_000_29266	AsGeYb	3	-3.883	-4.106	0.000e+00	0.00657	0.73	0.761
tri_000_29271	GeRhYb	3	-4.992	-5.147	-2.000e-06	0.00982	0.505	0.489
tri_000_29308	GaSiTb	3	-4.914	-4.936	-1.300e-05	0.00362	0.101	0.094
tri_000_29318	ClLiSTb	4	-0.724	-4.735	2.000e-06	0.00469	0.821	1.583
tri_000_29331	PmSiTb	3	-4.664	-5.19	-4.000e-06	0.00645	0.437	0.503
tri_000_29334	NdTl	2	-3.645	-3.692	-1.400e-06	0.00442	0.146	0.146
tri_000_29358	CaGd	2	-3.128	-3.146	-7.000e-07	0.00248	0.175	0.142
tri_000_29371	SeYb	2	-1.825	-4.246	-6.000e-07	0.00448	0.832	0.655
tri_000_29377	HFTb	3	-2.963	-5.172	-4.000e-06	0.00854	1.274	1.356
tri_000_29386	PrTb	2	-4.606	-4.619	-1.080e-05	0.00325	0.076	0.044
tri_000_29402	GdS ₂ Y	4	-0.619	-6.653	-2.000e-06	0.00382	1.649	1.638
tri_000_29442	BrTbV	3	-4.832	-5.077	-9.000e-06	0.00503	0.451	0.529
tri_000_29443	FeNdTe	3	-5.214	-5.778	-3.000e-06	0.00542	1.138	1.177
tri_000_29478	NiW	2	-8.97	-9.08	0.000e+00	0.00249	0.235	0.242
tri_000_29491	RuV	2	-9.056	-9.163	1.000e-05	0.00705	0.289	0.245
tri_000_29493	NdTb	2	-4.593	-4.613	-5.900e-06	0.00063	0.109	0.067
tri_000_29512	DyTb	2	-2.181	-4.354	-6.000e-07	0.00623	0.737	0.403

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_29564	Pt ₂ SbYb	4	-4.807	-5.159	0.000e+00	0.00312	0.528	0.47
tri_000_29572	DyNd	2	-4.498	-4.593	-2.000e-07	0.00232	0.223	0.163
tri_000_29598	AsCaMn	3	-4.959	-5.404	0.000e+00	0.00559	0.646	2.345
tri_000_29613	NbRu	2	-9.113	-9.772	-5.000e-06	0.00151	0.203	0.152
tri_000_29616	AuYb	2	-3.131	-3.155	-3.100e-06	0.00223	0.167	0.112
tri_000_29636	AuCuGdSe	4	-3.85	-4.449	0.000e+00	0.00544	1.033	1.351
tri_000_29649	PtSiYb	3	-5.25	-5.317	-2.000e-06	0.00399	0.216	0.173
tri_000_29672	H ₂ Ni	3	-3.62	-4.001	-1.400e-05	0.00444	0.653	1.636
tri_000_29680	H ₂ TbTi	4	-4.458	-4.944	0.000e+00	0.00541	1.267	0.503
tri_000_29684	BOsTb	3	-7.729	-7.871	1.000e-06	0.00146	0.291	0.312
tri_000_29688	Cd ₃ Mn	4	-1.795	-2.328	-2.600e-06	0.00761	0.465	0.473
tri_000_29696	Si ₂ Tb	3	-5.516	-5.681	1.000e-06	0.00516	0.337	0.409
tri_000_29712	DyZn	2	-2.774	-2.872	-1.702e-04	0.00797	0.482	0.306
tri_000_29717	Pd ₂ SbTb	4	-5.405	-5.502	0.000e+00	0.00731	0.355	0.289
tri_000_29732	EuYb	2	-1.626	-1.642	-2.100e-06	0.00287	0.236	0.151
tri_000_29747	H ₂ Dy	3	-4.326	-4.432	-4.000e-06	0.00031	0.152	0.144
tri_000_29764	AsCoDy	3	-5.732	-6.259	-3.900e-05	0.00713	0.579	0.779
tri_000_29806	B ₂ Ru	3	-7.321	-7.592	-2.000e-06	0.00662	0.834	0.28
tri_000_29807	SiSnYb	3	-3.511	-3.846	-1.000e-06	0.00561	0.457	0.468
tri_000_29823	Br ₂ Ru	3	-3.055	-4.002	0.000e+00	0.0094	1.146	1.303
tri_000_29845	MoSeTb	3	-6.002	-6.614	-1.000e-06	0.00531	2.446	4.502
tri_000_29854	BiNdPd ₂	4	-5.338	-5.364	0.000e+00	0.00355	0.214	0.163
tri_000_29881	MnPd	2	-6.552	-6.804	-1.000e-06	0.00514	0.397	0.389
tri_000_29890	CBMn	3	-7.95	-8.278	-1.000e-06	0.00339	0.344	0.626
tri_000_29900	CoNdRhSn	4	-5.716	-5.929	-1.200e-05	0.00797	0.51	0.399
tri_000_29909	NiPd	2	-5.009	-5.195	-6.000e-06	0.00431	0.252	0.207
tri_000_29918	CDy	2	-5.652	-6.785	0.000e+00	0.00168	1.32	2.016
tri_000_29931	HgTb	2	17.523	-2.5	-9.000e-07	0.00378	0.763	1.174
tri_000_29951	FeIr	2	-8.382	-8.518	-4.000e-06	0.00337	0.195	0.205
tri_000_29953	H ₂ Ni	3	-2.719	-4.0	-4.000e-06	0.00309	0.326	1.183
tri_000_29958	RuTb	2	-6.713	-6.897	-3.000e-06	0.00153	0.607	0.696
tri_000_29987	AlDySr	3	-2.638	-3.241	-5.000e-07	0.00503	1.145	1.027
tri_000_30024	NdSm	2	-4.632	-4.654	-1.400e-06	0.00368	0.166	0.195
tri_000_30029	DyGeMgRu	4	-4.626	-5.018	-3.000e-06	0.00755	0.552	2.108
tri_000_30034	GeNdNiSn	4	-4.882	-5.026	-3.400e-05	0.00643	0.152	0.18
tri_000_30040	CeDy	2	-5.023	-5.122	-2.300e-05	0.00893	0.317	0.178
tri_000_30047	LiO ₂ Ru	4	-5.792	-6.411	-2.000e-06	0.00454	0.335	1.042
tri_000_30052	FePd	2	-6.252	-6.332	-1.400e-05	0.00326	0.195	0.127
tri_000_30066	CoRh	2	-6.857	-6.96	2.000e-06	0.00148	0.132	0.107
tri_000_30075	CNdSb	3	-5.523	-5.885	1.000e-06	0.00874	0.555	0.518
tri_000_30096	FeNi	2	-6.412	-6.659	-8.000e-06	0.00345	0.457	0.459
tri_000_30172	RuZn	2	-4.835	-5.081	-8.700e-05	0.0028	0.252	0.157
tri_000_30188	GdTm	2	-4.406	-4.52	-9.000e-07	0.00163	0.287	0.138
tri_000_30208	AuFe	2	-4.789	-5.035	-4.000e-06	0.00633	0.206	0.126
tri_000_30239	AcNd	2	-4.305	-4.334	-7.000e-07	0.00172	0.175	0.178
tri_000_30246	BaNdSi	3	-3.969	-4.215	1.000e-06	0.00846	0.325	0.199
tri_000_30256	OsRu	2	-9.43	-10.107	-1.000e-06	0.00276	0.498	0.451
tri_000_30262	B ₂ Ru	3	-7.289	-7.605	0.000e+00	0.00403	0.879	0.328
tri_000_30296	GdNSi ₂	4	-5.649	-6.455	-6.000e-06	0.00885	0.713	1.42
tri_000_30303	CDyTe	3	-5.083	-5.572	-2.000e-06	0.00658	1.038	1.169
tri_000_30362	CoTc	2	-8.31	-8.604	-6.000e-06	0.00447	0.214	0.239
tri_000_30386	NiRh	2	-5.97	-6.254	-3.000e-06	0.00425	0.259	0.173

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_30427	LuTb	2	-4.494	-4.496	2.591e-02	0.00575	0.045	0.03
tri_000_30430	AsFeNdRh	4	-6.074	-6.398	-3.000e-06	0.00871	1.314	1.121
tri_000_30438	HGdSe	3	-4.323	-5.258	-2.000e-06	0.00384	1.265	1.115
tri_000_30451	TeVYb	3	-4.053	-4.523	4.000e-06	0.00532	0.532	0.548
tri_000_30458	Br ₂ Dy	3	-0.311	-4.206	0.000e+00	0.00486	0.425	1.276
tri_000_30476	CGd	2	-6.23	-6.432	-7.000e-06	0.00154	0.275	0.076
tri_000_30482	AuMn	2	-5.253	-5.472	-3.000e-06	0.0021	0.33	0.385
tri_000_30492	NdSn	2	-4.612	-4.755	-3.900e-06	0.0058	0.588	0.379
tri_000_30508	CGdPd	3	-5.734	-6.574	0.000e+00	0.00495	1.641	1.044
tri_000_30515	HgTb	2	-2.576	-2.69	-4.000e-07	0.00097	0.234	0.244
tri_000_30549	TbTe ₂	3	-4.498	-4.585	1.000e-06	0.00537	0.436	0.495
tri_000_30574	LuNd	2	-4.538	-4.539	-2.100e-06	0.00606	0.021	0.025
tri_000_30612	GdSiZn	3	-4.253	-4.355	-1.000e-06	0.00365	0.2	0.17
tri_000_30619	IrMn	2	-8.417	-8.942	-3.000e-06	0.00173	0.512	0.42
tri_000_30626	Se ₂ Tb	3	-4.679	-5.239	-1.000e-05	0.00531	0.839	1.002
tri_000_30659	CuTbTe	3	-3.792	-4.48	-4.000e-06	0.00526	0.886	2.432
tri_000_30665	Bi ₂ GdPd	4	-4.812	-4.865	-7.000e-06	0.00411	0.206	0.286
tri_000_30677	DySe ₂ Ti	4	-6.053	-6.161	0.000e+00	0.00431	0.257	1.104
tri_000_30685	FeZn ₂	3	-3.199	-3.278	4.000e-07	0.00261	0.429	0.418
tri_000_30689	PdRu	2	-6.889	-6.981	-2.000e-06	0.00138	0.149	0.118
tri_000_30700	DyTh	2	-5.909	-5.936	2.000e-06	0.00755	0.169	0.191
tri_000_30722	AsCdGd	3	-3.637	-3.962	-1.000e-06	0.00555	0.39	0.272
tri_000_30729	GaIrYb	3	-4.725	-5.019	-3.000e-06	0.00677	0.245	1.55
tri_000_30765	AuNdTe	3	-4.433	-4.65	0.000e+00	0.00549	0.646	0.65
tri_000_30795	AlGeTb	3	-4.806	-4.893	2.000e-06	0.00309	0.219	0.24
tri_000_30799	DyF ₂	3	-5.785	-6.147	0.000e+00	0.00802	0.449	0.312
tri_000_30815	PtSnTb	3	-5.277	-5.775	-4.000e-05	0.00573	1.099	0.789
tri_000_30834	CTbTe	3	-5.029	-5.586	0.000e+00	0.00478	0.88	0.93
tri_000_30847	GeTbZn	3	-4.03	-4.047	0.000e+00	0.0052	0.1	0.102
tri_000_30910	CoSeTb	3	-5.417	-5.952	-1.280e-04	0.00896	0.705	0.62
tri_000_30911	GdRhTe	3	-5.454	-5.971	-1.000e-06	0.00559	0.916	2.24
tri_000_30930	CeYb	2	-3.282	-3.446	5.500e-06	0.00268	0.53	0.404
tri_000_30933	NdZr	2	-6.315	-6.399	-1.000e-06	0.00417	0.297	0.155
tri_000_30939	Ni ₂	2	-5.359	-5.385	1.000e-06	0.00389	0.135	0.085
tri_000_30944	EuYb	2	-1.631	-1.642	-1.900e-06	0.00057	0.13	0.202
tri_000_30945	BrClDy	3	-3.992	-4.191	-3.000e-06	0.00505	0.546	0.343
tri_000_30974	NdRhSn	3	-5.717	-5.968	-1.000e-06	0.00532	0.592	0.655
tri_000_30983	NiZr	2	-6.722	-7.111	-2.300e-05	0.00491	0.909	0.871
tri_000_30993	LuNd	2	-4.528	-4.539	-1.300e-06	0.00104	0.112	0.099
tri_000_31020	DyErZn	3	-2.424	-3.488	1.300e-05	0.0042	1.456	1.311
tri_000_31057	ErYb	2	3.231	-2.695	7.000e-07	0.00184	1.212	0.966
tri_000_31112	Se ₂ Tb	3	-5.048	-5.246	0.000e+00	0.00279	0.924	0.88
tri_000_31115	H ₂ Co	3	-3.77	-4.485	0.000e+00	0.00601	0.44	1.395
tri_000_31148	AlBRu	3	-6.463	-6.573	0.000e+00	0.00947	0.067	0.14
tri_000_31151	CoRu	2	-7.841	-7.962	-7.000e-06	0.00282	0.114	0.043
tri_000_31155	MnPd	2	-6.45	-6.81	-4.000e-06	0.00343	0.546	0.529
tri_000_31159	CoPYb	3	-5.459	-5.493	-3.000e-06	0.00275	0.144	0.164
tri_000_31197	CdMnPd	3	-4.313	-4.636	-5.800e-05	0.00687	0.273	0.27
tri_000_31201	CoOs	2	-8.666	-8.992	-6.000e-06	0.00926	0.237	0.244
tri_000_31205	BiGdRh	3	-5.642	-5.857	-1.000e-06	0.00627	0.719	0.713
tri_000_31230	TIYb	2	-2.111	-2.151	-1.310e-05	0.00238	0.267	0.295
tri_000_31236	BeFeIr	3	-6.692	-6.898	-2.000e-06	0.0043	0.298	0.439

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_31249	CSbTb	3	-5.576	-5.881	-7.000e-06	0.00652	0.551	0.385
tri_000_31258	DyPtSe	3	-5.643	-5.828	0.000e+00	0.00331	0.57	0.712
tri_000_31282	CLiTb	3	-3.27	-5.085	-2.000e-06	0.00523	0.686	0.541
tri_000_31329	GdTm	2	-4.486	-4.524	-1.300e-06	0.00269	0.144	0.067
tri_000_31331	RuZn	2	-5.01	-5.068	-7.000e-06	0.00119	0.157	0.171
tri_000_31357	GaSiYb	3	-3.614	-3.76	-1.900e-05	0.00476	0.36	0.409
tri_000_31390	DyMgP	3	-4.176	-4.515	-1.000e-06	0.00356	0.364	0.393
tri_000_31405	CoPdSb	3	-5.139	-5.452	-2.000e-06	0.00753	1.143	1.284
tri_000_31412	CuIrNd	3	-5.639	-6.123	-3.000e-06	0.00287	0.773	0.682
tri_000_31499	TbTm	2	-4.491	-4.512	0.000e+00	0.00136	0.125	0.109
tri_000_31513	Dy ₂ Ge	3	-4.574	-4.957	-5.000e-06	0.00427	0.798	0.667
tri_000_31549	IrYbZr	3	-6.439	-6.586	-5.000e-05	0.00746	0.3	0.414
tri_000_31623	GaNd	2	-4.075	-4.096	1.400e-06	0.00146	0.21	0.181
tri_000_31658	NiZn	2	-3.341	-3.431	-3.000e-07	0.00428	0.219	0.18
tri_000_31670	TbTm	2	-4.488	-4.509	-3.000e-07	0.00093	0.123	0.136
tri_000_31672	CoGdSb	3	-5.274	-5.816	-2.800e-05	0.00914	0.91	0.673
tri_000_31686	GeNdTe	3	-4.206	-4.52	-3.000e-06	0.00789	0.659	0.827
tri_000_31697	NdTe	2	-4.731	-5.296	0.000e+00	0.00218	0.772	0.465
tri_000_31700	CoPt	2	-5.774	-6.354	-2.800e-05	0.00992	0.271	0.304
tri_000_31789	DyYb	2	-2.863	-2.887	6.000e-07	0.00063	0.162	0.22
tri_000_31799	CoOs	2	-8.729	-8.991	-3.000e-06	0.00044	0.131	0.072
tri_000_31812	EuYb	2	-1.631	-1.642	0.000e+00	0.00189	0.132	0.117
tri_000_31815	Cl ₂ Tb	3	-4.564	-4.676	1.000e-06	0.00736	0.191	0.175
tri_000_31830	B ₂ Ru	3	-7.218	-7.584	-6.000e-06	0.0053	0.734	0.921
tri_000_31843	MnPt	2	-7.03	-7.449	-1.100e-05	0.0077	0.462	0.391
tri_000_31862	FeTe	2	-2.443	-4.673	-2.300e-06	0.00414	4.098	6.282
tri_000_31873	B ₂ Ru	3	-7.046	-7.548	-1.000e-06	0.0042	0.722	0.851
tri_000_31897	AsCuNd	3	-4.762	-5.274	-1.900e-05	0.00943	0.45	0.592
tri_000_31910	CoOs	2	-8.584	-8.99	-2.000e-06	0.00266	0.292	0.217
tri_000_31915	NdNiP	3	-6.21	-6.343	-4.000e-06	0.0043	0.231	0.275
tri_000_31924	MnZn	2	-4.652	-4.789	-2.000e-06	0.00702	0.235	0.233
tri_000_31925	DyNd	2	-4.55	-4.594	-5.400e-06	0.00369	0.228	0.308
tri_000_31927	NdTe ₂ Ti	4	-5.319	-5.642	0.000e+00	0.00436	0.358	1.135
tri_000_31948	RuZr	2	-8.899	-8.971	-5.000e-06	0.00664	0.21	0.232
tri_000_31973	CaGd	2	-3.119	-3.145	-1.390e-05	0.00491	0.164	0.131
tri_000_32002	Be ₂ DyGe	4	4.982	-4.221	-1.000e-06	0.00865	0.885	1.248
tri_000_32036	CoLi	2	-3.661	-4.269	6.400e-06	0.00227	0.433	0.223
tri_000_32066	DyTe	2	-4.557	-5.098	-3.600e-05	0.00334	0.681	0.609
tri_000_32075	MoNi	2	-7.664	-8.127	0.000e+00	0.00547	0.803	0.806
tri_000_32078	NiRu	2	-7.064	-7.19	-6.000e-06	0.00327	0.152	0.105
tri_000_32088	LiO ₂ Ru	4	-6.271	-6.44	-5.000e-06	0.00855	0.287	0.21
tri_000_32092	Br ₂ Dy	3	-3.855	-4.207	-3.000e-06	0.00791	0.371	0.287
tri_000_32094	Rh ₂ SbYb	4	-5.447	-5.495	-8.000e-06	0.00476	0.265	0.272
tri_000_32108	MnTi	2	-8.172	-8.449	-4.100e-05	0.00581	0.204	0.2
tri_000_32111	DyPr	2	-4.599	-4.602	1.000e-06	0.00305	0.084	0.061
tri_000_32140	GdSm	2	-4.581	-4.599	-3.300e-06	0.00066	0.13	0.13
tri_000_32143	BeDySi	3	-5.128	-5.227	-1.000e-06	0.00346	0.215	0.155
tri_000_32164	CoRu	2	-7.786	-7.964	1.100e-05	0.00347	0.148	0.104
tri_000_32165	GdNd	2	-4.597	-4.629	8.700e-06	0.00758	0.196	0.109
tri_000_32167	NiV	2	-7.166	-7.257	-1.000e-05	0.00459	0.145	0.095
tri_000_32177	CrNdSSi	4	6.095	-6.163	1.000e-06	0.00327	1.108	1.902
tri_000_32208	NiPdRu	3	-6.084	-6.48	-3.000e-06	0.0066	0.218	0.183

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_32270	H ₂ Mn	3	-3.852	-5.113	-7.000e-06	0.00113	0.357	0.631
tri_000_32297	CTb	2	-5.492	-6.782	0.000e+00	0.00244	1.077	1.642
tri_000_32315	GeNdSr	3	-3.747	-3.936	-3.000e-06	0.0076	0.323	0.168
tri_000_32316	H ₂ Ni	3	-3.974	-4.045	-1.000e-06	0.00709	0.387	0.647
tri_000_32326	Se ₂ Tb	3	-4.727	-5.237	-1.200e-05	0.00763	0.883	0.775
tri_000_32344	CTbTe	3	-5.19	-5.594	-7.000e-06	0.00846	0.87	0.869
tri_000_32345	AuMn	2	-5.255	-5.472	-1.000e-06	0.00219	0.308	0.324
tri_000_32360	AuTeYb	3	-3.192	-3.46	-4.000e-06	0.003	0.917	1.135
tri_000_32361	PTb	2	0.551	-6.467	-3.000e-06	0.00191	1.887	1.375
tri_000_32393	AuMn	2	-5.232	-5.472	-1.000e-06	0.0015	0.322	0.234
tri_000_32418	CdRu	2	-4.393	-4.508	-2.000e-07	0.00295	0.541	0.608
tri_000_32424	GdGeMg	3	-3.31	-4.018	-8.000e-06	0.00614	0.223	0.756
tri_000_32431	Ru ₂	2	-9.071	-9.249	0.000e+00	0.00575	0.143	0.071
tri_000_32442	CdYb	2	-1.311	-1.33	-7.800e-06	0.00205	0.133	0.084
tri_000_32468	AlCdFe	3	-3.319	-3.974	0.000e+00	0.00372	0.71	0.553
tri_000_32483	GdTb	2	-4.513	-4.562	-8.700e-06	0.00087	0.209	0.095
tri_000_32503	GdTb	2	-4.512	-4.563	5.000e-06	0.00489	0.245	0.331
tri_000_32548	RuSiTe	3	3.288	-5.32	-1.000e-05	0.00912	0.732	2.117
tri_000_32562	IrRu	2	-8.678	-9.089	-3.000e-06	0.00373	0.292	0.204
tri_000_32636	Nd ₂	2	-4.665	-4.685	-8.900e-06	0.00019	0.176	0.249
tri_000_32653	IrMn	2	-8.933	-9.049	-1.800e-05	0.00359	0.153	0.126
tri_000_32688	GePTb	3	-5.358	-5.434	0.000e+00	0.00363	0.269	0.19
tri_000_32737	F ₂ Nd	3	-5.479	-5.995	-2.000e-06	0.00231	0.275	0.172
tri_000_32750	SbTb	2	-4.918	-5.257	-1.000e-06	0.00541	0.882	0.892
tri_000_32760	Cl ₂ Gd	3	-4.596	-4.698	-1.000e-06	0.00934	0.195	0.23
tri_000_32789	CaTb	2	-3.109	-3.122	7.000e-07	0.00241	0.116	0.081
tri_000_32795	BeSiYb	3	-3.864	-3.89	0.000e+00	0.00126	0.139	0.116
tri_000_32802	CdCo	2	-2.734	-3.334	4.000e-07	0.00511	0.327	0.208
tri_000_32836	BCoPt	3	-6.406	-6.764	0.000e+00	0.00889	0.8	0.979
tri_000_32857	HLiNiSi	4	0.537	-3.973	-1.000e-06	0.0098	1.015	1.487
tri_000_32877	NiPt	2	-5.287	-5.797	0.000e+00	0.00264	0.537	0.37
tri_000_32879	BeSiTb	3	-5.095	-5.233	1.000e-06	0.00431	0.204	0.211
tri_000_32880	GdY	2	-5.485	-5.507	5.000e-06	0.00043	0.139	0.188
tri_000_32896	Fe ₂ V ₂	4	-8.417	-8.629	-1.700e-05	0.00365	0.705	1.052
tri_000_32909	CoGdGeV	4	-5.876	-6.087	0.000e+00	0.00769	0.443	0.37
tri_000_32912	MnPt ₂	3	-6.429	-7.057	-6.000e-06	0.00555	0.487	0.44
tri_000_32913	DyPr	2	-4.588	-4.603	3.500e-06	0.00336	0.143	0.119
tri_000_32948	Au ₂ Gd ₂	4	-4.612	-4.667	-1.000e-06	0.00269	0.426	0.399
tri_000_32987	Si ₂ Yb	3	-4.404	-4.464	0.000e+00	0.00286	0.145	0.11
tri_000_33041	MnRu	2	-8.863	-9.069	1.000e-06	0.00264	0.245	0.21
tri_000_33046	CoNdY	3	-5.624	-6.042	0.000e+00	0.00394	0.897	0.71
tri_000_33059	GdOTl	3	-5.503	-5.676	-3.000e-06	0.00462	0.474	0.324
tri_000_33062	CdNi	2	-2.613	-2.935	-2.400e-06	0.00541	0.418	0.303
tri_000_33063	IrRu	2	-8.848	-9.083	-1.000e-06	0.00174	0.2	0.165
tri_000_33071	SnYb	2	-3.028	-3.155	4.000e-07	0.00556	0.343	0.188
tri_000_33092	NiZr	2	-6.029	-7.03	-5.400e-05	0.00374	0.927	0.68
tri_000_33136	CsYb	2	-0.546	-0.879	1.270e-05	0.00065	0.91	1.096
tri_000_33185	GdTb	2	-4.508	-4.566	2.500e-06	0.0025	0.219	0.128
tri_000_33200	B ₂ Ru	3	-7.276	-7.391	-1.000e-06	0.00843	0.121	0.106
tri_000_33201	AsNdPt	3	-6.138	-6.392	-1.000e-06	0.00635	0.292	0.404
tri_000_33209	FeGa	2	-5.334	-5.525	-1.000e-06	0.00107	0.193	0.396
tri_000_33231	GdSn	2	-4.499	-4.855	8.000e-07	0.00208	0.982	0.481

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_33236	LuYb	2	-2.641	-2.806	5.000e-07	0.00081	0.485	0.345
tri_000_33238	Tb ₂	2	-4.51	-4.547	-1.000e-06	0.00142	0.197	0.104
tri_000_33241	GeTbTe	3	-3.514	-4.474	0.000e+00	0.00895	0.773	0.542
tri_000_33250	CoFe	2	-7.422	-7.487	1.000e-06	0.00418	0.11	0.052
tri_000_33257	AuBiTb	3	-4.419	-4.535	-8.000e-06	0.00309	0.399	2.016
tri_000_33273	FeIr	2	-8.346	-8.517	1.100e-05	0.0049	0.215	0.156
tri_000_33305	Tb ₂	2	-4.513	-4.552	-1.900e-06	0.0049	0.201	0.101
tri_000_33312	GdSV	3	-5.97	-6.554	0.000e+00	0.00537	0.469	0.449
tri_000_33316	HCaNi	3	-2.321	-3.513	-2.000e-06	0.00783	0.734	0.504
tri_000_33369	Bi ₂ DyNi	4	-4.592	-4.742	-1.100e-05	0.00557	0.276	0.362
tri_000_33370	AuRu	2	-5.272	-5.681	8.824e-02	0.00849	0.44	0.436
tri_000_33385	SbSiYb	3	-3.694	-3.968	-1.000e-06	0.00241	0.518	0.458
tri_000_33399	FeLu	2	-5.645	-5.867	-2.000e-06	0.00075	0.407	0.303
tri_000_33424	Gd ₂ Se ₂	4	-5.678	-5.769	0.000e+00	0.00282	0.228	0.184
tri_000_33428	CuNdPtSe	4	-4.57	-5.25	-4.000e-05	0.00963	1.206	1.476
tri_000_33435	LuTb	2	-4.373	-4.499	3.600e-06	0.00171	0.328	0.291
tri_000_33479	MoNi	2	-7.956	-8.071	-1.300e-05	0.00329	0.233	0.143
tri_000_33485	RhRu	2	-8.005	-8.224	1.000e-06	0.0009	0.235	0.291
tri_000_33490	EuYb	2	-1.632	-1.642	-1.000e-06	0.00146	0.171	0.193
tri_000_33568	AuDyO	3	-3.969	-5.865	-7.000e-06	0.00552	1.052	1.932
tri_000_33575	CoFe	2	-7.37	-7.488	-5.000e-06	0.00911	0.148	0.114
tri_000_33602	CaNdP	3	-3.265	-4.856	-2.000e-06	0.00255	0.789	0.779
tri_000_33612	BrClRu	3	-3.391	-4.369	0.000e+00	0.00854	0.859	0.653
tri_000_33623	B ₂ Ru	3	-6.98	-7.4	0.000e+00	0.00346	0.354	0.324
tri_000_33641	HgTb	2	-2.626	-2.688	-9.000e-07	0.00368	0.17	0.08
tri_000_33670	H ₂ Mn	3	-3.619	-5.113	-1.000e-06	0.00338	0.327	0.598
tri_000_33690	GaGeTb	3	-4.547	-4.612	-1.000e-06	0.00943	0.201	0.137
tri_000_33719	As ₂ CoDy	4	-5.907	-5.928	-1.500e-05	0.00393	0.097	0.099
tri_000_33743	NdSi ₂	3	-5.734	-5.757	0.000e+00	0.0031	0.173	0.089
tri_000_33772	NiOs	2	-7.828	-8.191	-1.180e-04	0.00327	0.242	0.132
tri_000_33781	Co ₂	2	-6.787	-6.822	-1.100e-05	0.00741	0.108	0.122
tri_000_33799	FeGdTe	3	-4.958	-5.732	-1.100e-05	0.0058	1.14	1.033
tri_000_33870	GdS ₂	3	-5.253	-5.838	-1.000e-06	0.00407	1.488	1.908
tri_000_33871	FeNa	2	-3.502	-3.727	-2.800e-06	0.00414	0.274	0.466
tri_000_33874	IrMn	2	-8.75	-9.047	0.000e+00	0.0072	0.253	0.193
tri_000_33881	Sr ₂ Yb	3	-1.459	-1.551	-1.090e-05	0.0055	0.409	0.44
tri_000_33887	DyTh	2	-5.928	-5.935	-1.464e-02	0.00216	0.082	0.117
tri_000_33905	AgMn	2	-4.699	-5.081	-1.000e-06	0.00239	0.29	0.332
tri_000_33929	CoNdTe	3	-5.136	-5.67	-1.700e-05	0.00782	0.763	0.791
tri_000_33932	RuZr	2	-8.131	-8.891	-7.000e-06	0.00707	0.335	0.244
tri_000_33938	MnNdTe ₂	4	-5.07	-5.517	-3.000e-06	0.00748	0.757	0.816
tri_000_33947	SnYb	2	-2.791	-3.158	-6.000e-07	0.00517	0.585	0.738
tri_000_33949	OPrRu	3	-1.591	-6.793	-1.000e-06	0.00414	0.77	0.688
tri_000_33950	HgTb	2	-2.623	-2.684	-2.100e-06	0.0012	0.173	0.306
tri_000_33953	DyMgS ₂	4	-4.555	-5.186	-5.000e-06	0.00362	0.541	0.87
tri_000_33974	RuS ₂	3	-5.56	-6.023	-1.000e-06	0.00405	0.546	0.426
tri_000_34027	GdLu	2	-4.335	-4.506	-2.000e-06	0.00427	0.334	0.183
tri_000_34031	DyNiS	3	-5.461	-5.899	1.000e-05	0.00646	0.515	0.565
tri_000_34071	NiRu	2	-6.988	-7.188	-2.000e-06	0.00547	0.205	0.198
tri_000_34073	AgMn	2	-4.589	-5.077	0.000e+00	0.00232	0.519	0.583
tri_000_34078	AlMoNi	3	-6.704	-6.94	-1.400e-05	0.00264	0.829	0.552
tri_000_34095	CaTb	2	-3.097	-3.122	-3.500e-06	0.00096	0.224	0.188

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_34098	RhSeTb	3	-5.632	-6.268	-1.000e-06	0.004	0.823	1.003
tri_000_34104	FeOs	2	-9.418	-9.649	-2.300e-05	0.00611	0.209	0.216
tri_000_34143	PdRu	2	-6.79	-6.981	-2.000e-06	0.00368	0.259	0.348
tri_000_34152	DyP	2	-4.191	-6.584	0.000e+00	0.00122	0.949	0.589
tri_000_34165	NiTh	2	-4.221	-6.475	-4.300e-05	0.00582	0.949	0.475
tri_000_34169	CGa ₂ Yb	4	-3.327	-4.092	-1.000e-06	0.00703	1.355	1.475
tri_000_34170	RbYb	2	-0.704	-0.975	-1.000e-07	0.00154	0.976	0.851
tri_000_34190	BrGdTe	3	-4.647	-4.693	-2.000e-06	0.00339	0.437	0.478
tri_000_34200	PdSrYb	3	-3.1	-3.247	6.000e-07	0.0056	0.398	0.365
tri_000_34201	MnRh	2	-8.007	-8.132	-3.000e-06	0.00167	0.171	0.178
tri_000_34202	CoV	2	-7.957	-7.975	-6.000e-06	0.00563	0.067	0.048
tri_000_34210	As ₂ MnNb	4	-7.177	-7.439	0.000e+00	0.00364	0.26	0.972
tri_000_34214	Br ₂ Tb	3	-4.128	-4.24	1.000e-06	0.00924	0.286	0.393
tri_000_34260	LaTb	2	-4.675	-4.679	1.000e-07	0.00319	0.075	0.083
tri_000_34274	Ni ₂	2	-5.341	-5.383	2.600e-05	0.00738	0.126	0.095
tri_000_34315	PrYb	2	-2.94	-3.049	-7.290e-05	0.0032	0.398	0.371
tri_000_34371	GdRuSe	3	-5.972	-6.524	-2.000e-06	0.00725	0.908	2.346
tri_000_34386	AlMn	2	-6.21	-6.426	-1.900e-05	0.00366	0.25	0.32
tri_000_34390	FeV	2	-8.447	-8.549	-2.100e-05	0.0055	0.351	0.275
tri_000_34408	Al ₂ NdSn	4	-3.607	-4.137	1.000e-06	0.00461	0.611	1.442
tri_000_34421	NdNiSe	3	-5.121	-5.624	-1.449e-02	0.00633	0.748	0.678
tri_000_34429	NdZr	2	-6.328	-6.401	-2.270e-04	0.00448	0.234	0.196
tri_000_34458	CCoTb	3	-6.98	-7.027	-1.700e-05	0.00723	0.167	0.1
tri_000_34470	IrNi	2	-6.496	-7.134	-1.200e-05	0.00551	0.487	0.475
tri_000_34505	RuZr	2	-8.892	-8.969	-6.000e-06	0.00511	0.276	0.255
tri_000_34509	Co ₂ Mo	3	-7.912	-8.047	-8.100e-05	0.00402	0.224	0.244
tri_000_34533	CoNdSbSi	4	-5.455	-5.732	-2.300e-05	0.00569	0.373	1.275
tri_000_34549	CMnTh	3	-8.041	-8.505	0.000e+00	0.0031	0.325	0.206
tri_000_34591	H ₃ Fe	4	-3.281	-4.285	-2.000e-06	0.00433	0.96	1.327
tri_000_34637	NiOs	2	-7.859	-8.192	4.000e-06	0.00635	0.299	0.253
tri_000_34647	EuNdSi	3	-3.776	-4.203	0.000e+00	0.00373	0.51	0.3
tri_000_34655	AlCo	2	-5.386	-5.706	-3.000e-06	0.00684	0.373	0.347
tri_000_34698	NdSn	2	-4.625	-4.954	2.000e-07	0.00102	0.786	0.405
tri_000_34710	CoIr	2	-7.472	-7.846	1.100e-05	0.00948	0.272	0.151
tri_000_34751	EuNd	2	-3.18	-3.211	-1.260e-05	0.00768	0.287	0.321
tri_000_34765	Gd ₂	2	-4.571	-4.577	-5.000e-07	0.00117	0.079	0.101
tri_000_34773	NdTb	2	-4.557	-4.614	8.000e-07	0.00247	0.295	0.338
tri_000_34776	CeGd	2	-5.115	-5.138	-1.040e-04	0.007	0.219	0.175
tri_000_34845	PdRuTcTi	4	-7.86	-8.224	-7.400e-05	0.00713	0.27	0.403
tri_000_34852	FeRu	2	-8.07	-8.5	0.000e+00	0.00294	0.52	0.532
tri_000_34862	LiNdTe ₂	4	-4.469	-4.525	-2.000e-06	0.00858	0.234	1.277
tri_000_34874	RuZr	2	-8.931	-8.971	-3.000e-06	0.00801	0.158	0.139
tri_000_34931	ErSiYb	3	-3.297	-3.988	-3.000e-06	0.00449	0.496	0.651
tri_000_34935	DyEr	2	-4.489	-4.508	8.800e-06	0.00108	0.136	0.1
tri_000_34947	AsPTb	3	-4.566	-5.621	-4.000e-06	0.00898	1.283	1.335
tri_000_34962	PaRu	2	-9.254	-9.35	-2.000e-06	0.0033	0.221	0.208
tri_000_34964	FeNi	2	-6.587	-6.658	-5.000e-06	0.00262	0.13	0.031
tri_000_34966	CoPt	2	-6.084	-6.356	-3.600e-05	0.0019	0.246	0.2
tri_000_35009	CNd	2	-6.228	-6.655	-1.000e-06	0.00205	0.681	0.577
tri_000_35018	GaNd	2	-3.963	-4.094	-1.940e-05	0.00445	0.456	0.513
tri_000_35020	GdGeS	3	-4.528	-5.134	-3.000e-06	0.00743	0.646	0.271
tri_000_35024	DyGa ₂	3	-4.031	-4.091	0.000e+00	0.00779	0.177	0.137

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_35027	Gd ₂	2	-4.568	-4.573	-1.250e-05	0.00107	0.06	0.072
tri_000_35033	CGdRh	3	-7.126	-7.23	0.000e+00	0.00919	0.36	0.281
tri_000_35054	AlMn	2	-6.199	-6.397	-1.400e-05	0.00132	0.32	0.113
tri_000_35072	GeNiYb	3	-4.404	-4.43	-1.000e-06	0.00464	0.215	0.261
tri_000_35077	OTbTl	3	-5.396	-5.669	0.000e+00	0.00602	0.386	0.432
tri_000_35146	DyY	2	-5.45	-5.484	0.000e+00	0.00081	0.166	0.221
tri_000_35156	RuTh	2	-8.106	-8.399	0.000e+00	0.00823	0.758	0.473
tri_000_35161	Fe ₂ Na	3	-5.089	-5.212	1.000e-06	0.00385	0.25	0.238
tri_000_35166	GdTb	2	-4.54	-4.564	-2.000e-07	0.00151	0.135	0.182
tri_000_35189	CBRu	3	-7.372	-8.113	0.000e+00	0.00476	0.568	0.55
tri_000_35231	CLiNd	3	-4.949	-5.092	-1.000e-06	0.0067	0.194	0.302
tri_000_35238	AlGaTb	3	-4.257	-4.309	0.000e+00	0.00348	0.166	0.068
tri_000_35249	CaYb	2	-1.654	-1.686	-3.200e-06	0.00264	0.217	0.152
tri_000_35253	CdNi	2	-2.176	-2.891	1.500e-06	0.00661	0.554	0.515
tri_000_35256	GdTh	2	-5.916	-5.964	-3.000e-06	0.00363	0.234	0.153
tri_000_35258	HGd	2	-4.097	-4.348	-5.000e-07	0.00398	0.615	0.719
tri_000_35268	Nd ₂	2	-4.647	-4.685	6.000e-07	0.00235	0.232	0.201
tri_000_35273	NdPtSe	3	-5.749	-5.925	-6.000e-06	0.00946	0.31	0.344
tri_000_35275	DySeTe	3	-4.818	-4.902	3.000e-06	0.0038	1.059	0.938
tri_000_35287	B ₂ Ru	3	-7.371	-7.395	0.000e+00	0.00502	0.1	0.056
tri_000_35296	PdRuZr	3	-7.291	-7.778	-1.000e-06	0.00616	0.721	0.622
tri_000_35328	Ru ₂	2	-9.138	-9.236	-5.000e-06	0.00545	0.114	0.091
tri_000_35359	NdSn	2	-4.392	-4.955	-9.900e-06	0.00165	0.759	0.686
tri_000_35375	GaSiYb	3	-3.687	-3.757	-2.200e-05	0.00593	0.201	0.118
tri_000_35380	EuYb	2	-1.628	-1.642	-1.000e-07	0.00185	0.162	0.135
tri_000_35405	IrNdSi	3	-5.772	-7.087	-1.300e-05	0.00703	0.807	0.981
tri_000_35411	AgTbTe ₂	4	-4.114	-4.296	0.000e+00	0.00778	0.261	0.219
tri_000_35452	NiTc	2	-7.783	-7.833	9.000e-06	0.00375	0.073	0.048
tri_000_35461	S ₂ Tb	3	-5.537	-5.833	-3.000e-06	0.0024	1.682	1.159
tri_000_35476	MnZr	2	-7.623	-8.458	-4.000e-06	0.00153	0.552	0.531
tri_000_35478	CAsTb	3	-5.697	-6.177	-1.000e-06	0.00239	0.629	0.686
tri_000_35542	RuSbYb	3	-4.997	-5.258	-7.000e-06	0.00419	0.933	1.005
tri_000_35553	FePt	2	-6.481	-6.961	-8.000e-06	0.00122	0.53	0.324
tri_000_35556	LiRu	2	-4.674	-5.387	-2.000e-06	0.00371	0.504	0.294
tri_000_35582	CoFeRe	3	-8.734	-8.997	-2.000e-06	0.00773	0.273	0.289
tri_000_35592	Ru ₂	2	-9.007	-9.247	-1.700e-05	0.00402	0.21	0.11
tri_000_35629	CdYb	2	-1.196	-1.332	-3.200e-06	0.0025	0.409	0.237
tri_000_35644	MnRu	2	-8.615	-8.954	-9.000e-06	0.00393	0.498	0.325
tri_000_35653	AuNiPt	3	-3.936	-4.851	-9.500e-05	0.00457	0.363	0.203
tri_000_35671	NdSi ₂	3	-5.622	-5.757	-2.000e-06	0.00449	0.197	0.331
tri_000_35681	HfMnRh	3	-8.28	-8.723	-2.000e-06	0.00902	0.761	0.573
tri_000_35718	NiV	2	-7.117	-7.258	2.000e-06	0.00532	0.23	0.177
tri_000_35735	NdPtSe	3	-5.539	-5.92	-1.000e-06	0.00318	0.741	0.882
tri_000_35752	AlCoZr	3	-5.608	-6.631	1.000e-06	0.00494	1.008	0.708
tri_000_35760	P ₂ Tb	3	-4.755	-5.835	0.000e+00	0.00369	0.537	0.726
tri_000_35768	GdNiSb	3	-5.233	-5.545	0.000e+00	0.00961	0.525	0.528
tri_000_35769	CeNd	2	-5.046	-5.185	0.000e+00	0.00079	0.337	0.188
tri_000_35774	NiOs	2	-7.862	-8.191	-3.000e-06	0.00425	0.223	0.161
tri_000_35789	IrRu	2	-8.949	-9.084	-5.000e-06	0.00401	0.193	0.137
tri_000_35837	Au ₂ Yb ₂	4	-3.048	-3.163	0.000e+00	0.00553	0.582	0.529
tri_000_35857	Ni ₂	2	-5.373	-5.386	-1.100e-05	0.00669	0.075	0.058
tri_000_35875	GeNdP	3	-5.157	-5.56	-2.000e-06	0.00459	0.519	0.318

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_35909	NdSm	2	-4.65	-4.654	-3.000e-07	0.00578	0.069	0.039
tri_000_35914	AlGeNd	3	-4.87	-5.003	-3.000e-06	0.00693	0.264	0.281
tri_000_35953	DyTe	2	27.439	-4.939	-2.300e-06	0.00442	1.022	1.147
tri_000_35988	CMnP ₂	4	-6.681	-7.252	-2.000e-06	0.00762	0.44	1.874
tri_000_36027	MnPd	2	-6.787	-6.827	-1.800e-05	0.00204	0.113	0.098
tri_000_36054	GeSiYb	3	-4.161	-4.184	-2.000e-06	0.00732	0.096	0.057
tri_000_36067	NdSiSm	3	-4.532	-5.358	-1.400e-05	0.00478	1.233	1.523
tri_000_36090	CDy ₂	3	-6.014	-6.38	-6.000e-06	0.00566	0.756	0.944
tri_000_36110	CeDy	2	-4.976	-5.124	1.000e-06	0.00215	0.368	0.224
tri_000_36144	FeZn	2	-4.367	-4.41	4.600e-06	0.00327	0.138	0.215
tri_000_36174	ErGd	2	-4.5	-4.529	-5.000e-07	0.0047	0.12	0.148
tri_000_36177	AsYb	2	-2.506	-4.015	-2.100e-06	0.00223	1.313	1.262
tri_000_36204	NdSn	2	-4.702	-4.751	-1.700e-06	0.00728	0.175	0.159
tri_000_36215	CBMn	3	-7.763	-8.273	0.000e+00	0.00532	0.558	0.535
tri_000_36222	CoRe	2	-9.34	-9.652	4.000e-06	0.00793	0.191	0.118
tri_000_36234	SnTb	2	-4.672	-4.684	-2.000e-06	0.00139	0.095	0.141
tri_000_36241	LuTb	2	-4.411	-4.496	4.000e-06	0.004	0.225	0.167
tri_000_36246	H ₂ Ni	3	-2.336	-3.997	-8.000e-06	0.00418	0.285	0.519
tri_000_36252	InYb	2	-2.233	-2.486	-1.620e-05	0.00784	0.929	0.887
tri_000_36258	GaTbY	3	-4.281	-4.873	-8.000e-06	0.00647	0.554	0.645
tri_000_36279	NdTh	2	-5.943	-6.002	-3.000e-06	0.00444	0.261	0.221
tri_000_36301	GdSn	2	-4.598	-4.708	8.000e-07	0.00945	0.223	0.092
tri_000_36307	Ni ₂ SnYb	4	-4.324	-4.337	-5.000e-06	0.00501	0.066	0.064
tri_000_36338	TbTl	2	-0.775	-3.421	-1.600e-06	0.00254	0.688	0.402
tri_000_36366	Co ₂ GdSn	4	-5.569	-5.717	-3.900e-05	0.0073	0.479	0.369
tri_000_36369	PrYb	2	-2.985	-3.049	2.600e-06	0.00308	0.296	0.289
tri_000_36387	CdTb	2	-2.731	-2.76	-8.000e-07	0.00226	0.148	0.051
tri_000_36459	NdTe ₂	3	-4.491	-4.723	1.000e-06	0.00589	1.129	0.985
tri_000_36468	MnSc	2	-6.854	-7.214	-2.000e-06	0.00061	0.453	0.532
tri_000_36487	DyIn	2	11.1	-3.694	-7.000e-07	0.00584	0.827	3.005
tri_000_36498	AlNi	2	-4.858	-5.165	-1.000e-06	0.00503	0.737	0.72
tri_000_36535	AuFe	2	-4.694	-5.033	1.000e-06	0.00395	0.313	0.193
tri_000_36536	GdP ₂	3	-3.82	-5.933	-3.000e-06	0.00446	0.744	0.641
tri_000_36563	HHfRu	3	-7.571	-7.689	1.100e-05	0.00467	0.408	0.664
tri_000_36565	AcGd	2	-4.225	-4.249	-3.000e-06	0.00269	0.197	0.196
tri_000_36575	CoPt	2	-6.039	-6.355	-3.000e-06	0.00715	0.218	0.169
tri_000_36600	DyLu	2	-4.445	-4.489	-3.600e-06	0.00206	0.17	0.076
tri_000_36634	GdMg	2	-2.955	-2.986	-4.100e-06	0.00215	0.174	0.087
tri_000_36670	AuRu	2	-5.304	-5.664	1.000e-06	0.00166	0.501	0.296
tri_000_36722	DyPtSe	3	-5.565	-5.822	-1.000e-06	0.00451	0.719	0.663
tri_000_36753	AlDyTm	3	-3.919	-4.4	-1.000e-06	0.00151	0.889	0.919
tri_000_36764	AuMn	2	-5.124	-5.492	-2.000e-06	0.0006	0.518	0.605
tri_000_36767	CoIrPt	3	-6.883	-7.207	-6.000e-06	0.00415	0.236	0.41
tri_000_36774	HRuSi	3	-5.558	-6.036	-1.000e-06	0.00438	0.315	0.351
tri_000_36806	MnV	2	-8.863	-9.126	-5.000e-06	0.00155	0.348	0.262
tri_000_36810	NiPt	2	-5.515	-5.803	0.000e+00	0.0035	0.503	0.37
tri_000_36841	TbTm	2	-4.471	-4.509	-2.600e-06	0.00176	0.187	0.195
tri_000_36880	Cl ₂ Nd	3	-4.501	-4.757	0.000e+00	0.00222	0.352	0.273
tri_000_36890	AsGdPt	3	-6.273	-6.345	0.000e+00	0.00942	0.136	0.106
tri_000_36920	DySb	2	-5.169	-5.232	-2.000e-06	0.00202	0.226	0.191
tri_000_36922	AgGdS	3	-4.298	-4.685	-1.900e-05	0.00554	0.507	0.654
tri_000_36930	CBGd	3	-5.147	-7.069	0.000e+00	0.00245	1.239	1.341

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_37008	AuNdSe ₂	4	-4.261	-4.834	-1.000e-06	0.00512	0.626	0.415
tri_000_37058	OsRu	2	-9.287	-10.078	-2.000e-06	0.0068	0.518	0.572
tri_000_37079	NdSe ₂	3	-4.989	-5.366	-5.000e-06	0.00177	1.475	1.709
tri_000_37105	Nd ₂	2	-4.671	-4.685	-1.930e-05	0.00249	0.156	0.102
tri_000_37140	NdTe	2	-4.972	-5.298	-1.000e-06	0.00272	0.335	0.163
tri_000_37169	H ₃ Tb	4	-2.86	-4.23	-1.000e-06	0.0016	0.402	0.868
tri_000_37220	DyPr	2	-4.575	-4.602	-1.200e-06	0.00078	0.141	0.075
tri_000_37224	Fe ₂ Zn	3	-5.496	-5.69	1.000e-06	0.00882	0.587	0.707
tri_000_37303	PtRu	2	-7.393	-7.54	-3.000e-06	0.00581	0.177	0.151
tri_000_37327	CoEr	2	-4.027	-5.602	0.000e+00	0.00184	1.047	0.708
tri_000_37360	DyPtTe	3	-4.836	-5.588	0.000e+00	0.00247	0.27	0.718
tri_000_37379	MnRe	2	-10.218	-10.553	-9.000e-06	0.00713	0.439	0.383
tri_000_37431	CBRu	3	-7.428	-8.139	0.000e+00	0.00707	0.669	0.505
tri_000_37434	MnPt	2	-7.07	-7.47	0.000e+00	0.00656	0.38	0.44
tri_000_37486	CoO ₂	3	-6.335	-6.475	-1.200e-05	0.00986	0.089	0.139
tri_000_37493	CoIrZr	3	-7.647	-8.204	1.000e-05	0.00831	0.909	0.638
tri_000_37506	AlGeYb	3	-3.7	-3.717	-2.000e-06	0.00427	0.096	0.07
tri_000_37530	MnRe	2	-10.235	-10.594	5.000e-06	0.00448	0.213	0.17
tri_000_37594	AuRu	2	-5.372	-5.736	-5.000e-06	0.00534	0.365	0.13
tri_000_37621	AlSbYb	3	-3.275	-3.537	0.000e+00	0.00368	0.38	0.314
tri_000_37658	EuNd	2	-3.161	-3.214	5.100e-06	0.00336	0.293	0.25
tri_000_37669	AgDyErLi	4	-2.254	-3.31	-1.000e-06	0.00874	0.835	0.454
tri_000_37681	AuMn	2	-5.289	-5.475	-1.000e-06	0.0024	0.409	0.555
tri_000_37685	GdNdSi	3	-4.945	-5.157	1.000e-06	0.00625	0.394	0.264
tri_000_37725	NdSn	2	-4.645	-4.958	-8.100e-06	0.00116	0.766	0.277
tri_000_37736	IrRu	2	-8.948	-9.087	-9.000e-06	0.0046	0.132	0.062
tri_000_37739	FeIr	2	-8.38	-8.516	-3.000e-06	0.00196	0.161	0.08
tri_000_37747	DySe ₂	3	-4.709	-5.231	-1.000e-06	0.00196	0.892	0.747
tri_000_37761	PRuSb	3	-5.556	-6.287	1.000e-06	0.00654	0.594	0.495
tri_000_37773	BRuSc	3	-7.384	-7.797	-7.000e-06	0.00746	0.271	0.327
tri_000_37777	EuYb	2	-1.632	-1.643	-3.800e-06	0.00058	0.144	0.104
tri_000_37815	GdGeTb	3	-4.248	-4.893	0.000e+00	0.00898	0.506	0.334
tri_000_37863	H ₂ Co	3	-2.87	-4.479	-2.200e-05	0.00512	0.419	0.559
tri_000_37873	MnRu	2	-8.993	-9.07	-6.000e-06	0.00767	0.126	0.123
tri_000_37892	PSiTb	3	-3.397	-5.743	-1.000e-06	0.00364	0.837	0.531
tri_000_37897	GaNd	2	-3.992	-4.099	-2.000e-06	0.00387	0.255	0.159
tri_000_37927	NdTm	2	-4.515	-4.555	8.500e-06	0.00229	0.134	0.217
tri_000_37936	BiGd	2	-4.644	-4.915	4.400e-06	0.00279	0.947	0.834
tri_000_37938	GePYb	3	-4.135	-4.373	-7.000e-06	0.00894	0.382	0.299
tri_000_37958	MnTc	2	-9.311	-9.557	-1.200e-05	0.00661	0.087	0.347
tri_000_37993	AlFe	2	-5.952	-6.132	0.000e+00	0.00252	0.19	0.342
tri_000_37996	CdNi	2	-2.217	-2.896	-7.200e-06	0.00303	0.46	0.302
tri_000_38022	LaNdSi	3	-4.491	-5.422	-1.000e-06	0.00764	0.972	0.856
tri_000_38042	GdMg	2	-2.879	-2.986	-1.000e-05	0.00151	0.365	0.154
tri_000_38052	BRuY	3	-6.737	-7.864	0.000e+00	0.00496	0.354	0.205
tri_000_38061	CGd	2	-6.348	-6.433	0.000e+00	0.00116	0.172	0.067
tri_000_38064	RuTm	2	-6.033	-6.778	-4.000e-06	0.00914	0.363	0.218
tri_000_38081	BaSiTb	3	-3.563	-4.19	0.000e+00	0.00403	0.52	0.304
tri_000_38087	RhTbTe	3	-5.214	-5.842	-1.000e-06	0.00973	1.06	0.994
tri_000_38093	AlDySi	3	-5.056	-5.169	-1.000e-06	0.00318	0.235	0.233
tri_000_38112	Sb ₂ Tb	3	-4.39	-4.833	-1.000e-06	0.00545	1.713	1.368
tri_000_38131	IrNbRhRu	4	-8.758	-8.953	-1.000e-06	0.00832	0.401	1.074

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_38150	BrTb	2	-1.628	-4.162	-1.000e-06	0.00236	0.571	0.78
tri_000_38155	FeLi	2	-4.602	-4.705	-4.000e-07	0.0021	0.201	0.092
tri_000_38217	SnYb	2	-2.641	-3.16	-1.200e-06	0.00432	0.632	0.46
tri_000_38234	AlGdSi	3	-4.959	-5.216	0.000e+00	0.003	0.348	1.561
tri_000_38255	CdTb	2	18.306	-2.774	-1.000e-07	0.00408	1.092	1.083
tri_000_38260	NiRu	2	-6.659	-7.173	0.000e+00	0.00597	0.526	0.433
tri_000_38261	Ru ₂	2	-9.045	-9.243	-7.000e-06	0.00214	0.203	0.228
tri_000_38288	NdSe ₂	3	-4.62	-5.369	1.000e-06	0.00361	1.43	1.375
tri_000_38294	DyTb	2	-4.536	-4.54	-1.000e-07	0.00116	0.057	0.049
tri_000_38318	DyEr	2	-4.504	-4.512	-1.310e-05	0.00622	0.106	0.087
tri_000_38381	TbTeTi	3	-5.081	-5.565	-4.000e-06	0.00295	0.637	0.53
tri_000_38415	CoI ₂	3	-3.152	-3.299	-2.000e-07	0.00473	0.244	0.142
tri_000_38420	AuFe	2	-4.903	-5.037	-1.700e-05	0.00337	0.144	0.19
tri_000_38457	CuFe	2	-5.497	-5.6	-2.000e-05	0.00547	0.224	0.211
tri_000_38467	AlAsRu	3	-5.539	-6.105	-5.000e-06	0.0041	0.294	0.24
tri_000_38473	DyTb	2	-2.03	-4.455	-4.000e-06	0.00185	0.674	1.181
tri_000_38482	CoOs	2	-8.225	-8.933	-1.000e-06	0.00608	0.521	0.25
tri_000_38483	ErNd	2	-4.527	-4.568	4.000e-07	0.0049	0.202	0.24
tri_000_38540	BeNdSi	3	-5.136	-5.22	-2.000e-06	0.00245	0.154	0.144
tri_000_38558	H ₂ Mn	3	-4.659	-4.848	-2.000e-06	0.00117	0.492	0.971
tri_000_38569	BrNdNi	3	-4.252	-4.467	-4.400e-05	0.0087	0.837	0.908
tri_000_38575	Ni ₂	2	-5.345	-5.384	-1.600e-05	0.00374	0.116	0.116
tri_000_38598	BeSiYb	3	-3.843	-3.891	-4.000e-06	0.00086	0.238	0.256
tri_000_38636	NdTe	2	-5.211	-5.299	2.000e-06	0.00336	0.209	0.166
tri_000_38637	Tb ₂	2	-4.533	-4.552	-3.700e-06	0.00176	0.125	0.073
tri_000_38638	FeRe	2	-9.87	-10.248	-9.000e-06	0.00526	0.334	2.505
tri_000_38657	GdSiTh	3	-5.606	-6.148	-3.000e-06	0.00209	1.326	0.771
tri_000_38686	Gd ₂ O	3	-6.469	-6.488	0.000e+00	0.00183	0.093	0.079
tri_000_38691	FeV	2	-8.467	-8.551	-3.000e-06	0.00188	0.279	0.298
tri_000_38700	AgRu	2	-4.922	-5.355	-1.000e-06	0.00339	0.381	0.449
tri_000_38716	CuPt ₂ Tb	4	-5.339	-5.489	-1.600e-05	0.00708	0.321	1.208
tri_000_38744	CoIr	2	-7.634	-7.839	-1.000e-06	0.00456	0.235	0.285
tri_000_38762	H ₂ NdV	4	-3.73	-5.099	-1.800e-05	0.00616	0.865	0.833
tri_000_38767	CoNi	2	-6.047	-6.057	-2.300e-05	0.0079	0.044	0.049
tri_000_38786	AsYb	2	-2.989	-4.035	3.000e-07	0.00515	1.103	0.876
tri_000_38808	CGdSb	3	-5.576	-5.885	-3.000e-06	0.00553	0.57	0.664
tri_000_38821	MnPt	2	-7.006	-7.455	-2.000e-06	0.00312	0.517	0.503
tri_000_38837	AuNi	2	-4.06	-4.142	-8.100e-06	0.00564	0.142	0.195
tri_000_38843	FeGa	2	-5.369	-5.52	1.000e-06	0.0024	0.254	0.213
tri_000_38853	HgLiRu	3	-3.24	-3.427	0.000e+00	0.00551	0.571	0.762
tri_000_38857	AuRu	2	-5.697	-5.713	-2.100e-05	0.00725	0.081	0.087
tri_000_38874	DyHo	2	-4.503	-4.516	-8.000e-07	0.00225	0.119	0.07
tri_000_38879	DyIn	2	-3.816	-3.819	-8.300e-06	0.00592	0.034	0.019
tri_000_38901	MnOsZn	3	-6.799	-7.001	-3.000e-06	0.00433	0.217	0.261
tri_000_38944	GaPtYb	3	-4.224	-4.428	-9.000e-06	0.00417	0.452	0.402
tri_000_38962	AlGdGe	3	-4.755	-4.916	1.000e-06	0.00443	0.284	0.191
tri_000_38964	CoIr	2	-7.693	-7.84	0.000e+00	0.00371	0.163	0.126
tri_000_38988	GaYb	2	-2.379	-2.428	1.000e-07	0.00722	0.21	0.137
tri_000_39006	Cl ₂ Dy	3	-4.507	-4.651	-8.000e-06	0.00545	0.369	0.459
tri_000_39010	CDySi	3	-6.231	-6.462	0.000e+00	0.00634	0.532	0.45
tri_000_39014	DySSe	3	-4.875	-5.526	-2.000e-06	0.0078	0.791	1.823
tri_000_39027	GaGdSi	3	-4.608	-4.963	-3.000e-06	0.00641	0.386	0.366

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_39032	TeYb	2	-3.352	-3.817	-8.500e-06	0.00371	0.616	0.429
tri_000_39052	NbRu	2	-9.44	-9.683	0.000e+00	0.00669	0.173	0.149
tri_000_39081	EuYb	2	-1.626	-1.643	2.100e-06	0.00183	0.244	0.298
tri_000_39129	FeNi	2	-6.449	-6.656	5.000e-06	0.00223	0.295	0.314
tri_000_39132	NbRu	2	-9.313	-9.777	-1.200e-05	0.00128	0.258	0.112
tri_000_39154	AsNiTb	3	-5.557	-5.959	-1.600e-05	0.00622	0.359	0.451
tri_000_39171	GdSi ₂	3	-5.363	-5.702	-4.000e-06	0.00159	0.343	0.534
tri_000_39174	GaNdPd	3	-4.871	-5.081	-3.000e-06	0.0032	0.445	0.486
tri_000_39183	AsMnTb	3	-6.144	-6.529	2.000e-06	0.00298	0.534	0.649
tri_000_39205	Ga ₂ Nd	3	-4.049	-4.201	-1.100e-05	0.00855	0.315	0.202
tri_000_39241	GdGeSr	3	-3.389	-3.919	-1.000e-06	0.00582	0.511	0.354
tri_000_39249	CuGdTe	3	-4.331	-4.516	-2.000e-06	0.00894	0.627	0.671
tri_000_39251	CrLiNTb	4	-6.134	-6.265	1.000e-06	0.0026	0.492	0.54
tri_000_39379	S ₂ TbYb	4	-5.191	-5.576	0.000e+00	0.00216	0.503	0.509
tri_000_39416	HDyGe	3	-4.143	-4.466	-1.600e-05	0.00908	0.22	0.705
tri_000_39419	FeOs	2	-9.413	-9.648	-3.900e-05	0.00228	0.189	0.185
tri_000_39434	NiRe	2	-8.81	-8.876	-6.900e-05	0.00826	0.099	0.066
tri_000_39469	GdSiZn	3	-3.753	-4.349	-1.000e-06	0.00605	0.715	2.354
tri_000_39496	GdTm	2	-4.43	-4.52	-6.000e-07	0.00464	0.224	0.113
tri_000_39501	NdTl	2	-3.655	-3.699	-6.900e-06	0.0035	0.258	0.22
tri_000_39535	AgGeSeTb	4	-3.788	-4.258	-2.000e-06	0.00693	0.497	0.301
tri_000_39595	Cl ₂ Dy	3	-4.288	-4.658	-2.000e-06	0.00724	0.565	0.748
tri_000_39620	CHMn	3	-6.027	-6.596	0.000e+00	0.00543	0.624	0.518
tri_000_39633	NdTb	2	-4.589	-4.609	-2.200e-06	0.00374	0.129	0.139
tri_000_39652	ErTb	2	-4.515	-4.52	1.300e-06	0.0031	0.059	0.05
tri_000_39688	IrMn	2	-8.489	-8.945	-3.100e-05	0.00208	0.526	0.424
tri_000_39690	IrRuSe ₂	4	-5.774	-6.104	-1.000e-06	0.00735	0.347	0.228
tri_000_39702	NiTc ₃	4	-8.062	-9.071	-1.680e-04	0.00566	0.533	0.562
tri_000_39753	FeIr	2	-8.434	-8.516	-1.000e-06	0.00163	0.124	0.12
tri_000_39794	FeRe	2	-9.904	-10.246	-5.000e-06	0.00587	0.256	0.213
tri_000_39822	DyMgSn	3	-3.112	-3.721	0.000e+00	0.00424	0.958	1.979
tri_000_39834	B ₂ Ru	3	-7.293	-7.399	-2.000e-06	0.00537	0.15	0.087
tri_000_39845	NiRh	2	-6.044	-6.254	0.000e+00	0.00541	0.232	0.125
tri_000_39870	I ₂ Nd	3	-3.784	-3.895	-9.000e-06	0.00403	0.286	0.131
tri_000_39886	NdPd ₂ Sn	4	-5.274	-5.535	0.000e+00	0.00511	0.344	0.311
tri_000_39888	CBRu	3	-7.193	-8.101	0.000e+00	0.00479	0.867	0.743
tri_000_39938	CoV	2	-7.963	-7.976	1.000e-06	0.00666	0.05	0.031
tri_000_39980	CoV	2	-7.917	-7.974	3.000e-06	0.00314	0.093	0.096
tri_000_40068	CTbV	3	-7.184	-7.639	-2.000e-05	0.00659	0.709	0.512
tri_000_40093	SeTb	2	-5.676	-5.704	0.000e+00	0.00408	0.085	0.105
tri_000_40124	EuGd	2	-3.064	-3.11	5.000e-07	0.00228	0.319	0.221
tri_000_40145	BiTb	2	-4.645	-4.906	-4.780e-05	0.00894	0.755	0.511
tri_000_40173	GdS ₂	3	-5.298	-5.829	0.000e+00	0.00251	1.452	1.86
tri_000_40175	CeDy	2	-5.087	-5.115	-2.000e-06	0.00118	0.2	0.22
tri_000_40251	GdSm	2	-4.588	-4.603	6.000e-07	0.00221	0.111	0.075
tri_000_40260	AcTb	2	-4.221	-4.227	-2.500e-06	0.00267	0.09	0.113
tri_000_40262	B ₂ Ru	3	-7.355	-7.431	-4.000e-06	0.00252	0.279	0.257
tri_000_40265	As ₂ Ni ₂	4	-5.131	-5.353	-1.500e-05	0.00265	0.318	0.264
tri_000_40269	LiRu	2	-4.823	-5.386	-1.000e-06	0.00818	0.478	0.366
tri_000_40281	CoCr	2	-8.16	-8.17	-4.000e-06	0.00418	0.045	0.022
tri_000_40282	DySn	2	-4.543	-4.676	-5.900e-06	0.00207	0.507	0.302
tri_000_40285	NiRu	2	-7.054	-7.19	7.000e-06	0.00518	0.176	0.176

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_40305	FeRe	2	-9.827	-10.149	-7.900e-05	0.00426	0.482	0.349
tri_000_40324	MnW	2	-10.431	-10.665	-5.000e-06	0.00353	0.268	0.316
tri_000_40342	NiRe	2	-8.537	-8.875	3.000e-06	0.00555	0.129	0.045
tri_000_40343	CoGdSi	3	-6.043	-6.292	-4.800e-05	0.00858	0.291	0.235
tri_000_40348	AgNiSbYb	4	-3.702	-3.801	5.000e-06	0.00519	0.255	0.328
tri_000_40366	FeGdSe	3	-5.491	-6.086	-2.000e-06	0.00418	0.948	0.749
tri_000_40376	BRuTb	3	-6.35	-7.235	-1.000e-06	0.00398	0.437	0.417
tri_000_40407	AsCaTb	3	-3.582	-4.535	-4.000e-06	0.00548	0.654	0.849
tri_000_40413	AsInYb	3	-3.521	-3.579	-6.000e-06	0.00262	0.269	0.244
tri_000_40415	CuRu	2	-5.949	-6.186	0.000e+00	0.00325	0.532	0.498
tri_000_40445	Co ₂	2	-6.773	-6.822	-2.300e-05	0.00186	0.131	0.126
tri_000_40460	RhRu	2	-7.983	-8.234	-1.000e-06	0.00704	0.254	0.242
tri_000_40464	CaYb	2	-1.641	-1.685	-8.000e-07	0.0038	0.218	0.274
tri_000_40473	NdSb	2	-5.174	-5.384	-1.000e-06	0.00356	0.46	0.262
tri_000_40552	HgNi	2	-1.248	-2.467	-1.690e-05	0.00317	0.716	0.297
tri_000_40585	AuGaGd	3	-3.981	-4.374	-2.000e-06	0.00634	0.67	1.855
tri_000_40629	CuTb	2	-4.174	-4.189	-4.910e-05	0.00177	0.129	0.126
tri_000_40658	Gd ₂	2	-4.569	-4.579	-6.600e-06	0.00292	0.066	0.029
tri_000_40700	CaYb	2	-1.624	-1.685	-1.500e-06	0.00338	0.295	0.36
tri_000_40726	NdSi ₂	3	-5.274	-5.757	0.000e+00	0.00213	0.397	0.477
tri_000_40747	InYb	2	-2.246	-2.488	-5.500e-06	0.00135	0.936	0.376
tri_000_40764	AcNd	2	-4.256	-4.334	1.800e-06	0.00187	0.306	0.178
tri_000_40778	CDySn	3	-5.736	-5.761	1.000e-06	0.00538	0.331	0.242
tri_000_40791	NiRu	2	-7.106	-7.195	4.000e-06	0.00331	0.159	0.13
tri_000_40799	PSiYb	3	-4.335	-4.621	-3.000e-06	0.00357	0.389	0.295
tri_000_40826	MnPt ₂	3	-6.937	-7.068	-8.000e-06	0.00676	0.16	0.21
tri_000_40831	CuTe ₂ Yb	4	-3.322	-3.571	-4.650e-04	0.00743	0.422	0.254
tri_000_40857	Ni ₃	3	-5.369	-5.414	-3.100e-05	0.00366	0.178	0.152
tri_000_40858	GdPtS	3	-5.288	-6.132	0.000e+00	0.00487	1.066	0.92
tri_000_40865	CeGd	2	-5.108	-5.146	-2.000e-06	0.00782	0.145	0.066
tri_000_40900	GdP ₂	3	-4.038	-5.948	-1.000e-05	0.00313	0.498	0.541
tri_000_40921	CoRh	2	-6.84	-6.964	-1.000e-06	0.00483	0.155	0.098
tri_000_40932	CoFe	2	-7.403	-7.487	-1.000e-06	0.00485	0.136	0.086
tri_000_40944	CTb	2	-5.792	-6.46	-1.000e-06	0.00328	0.421	0.811
tri_000_40957	NiV	2	-7.257	-7.264	-1.800e-05	0.00929	0.047	0.056
tri_000_40962	PdRu	2	-6.697	-6.988	-1.300e-05	0.00519	0.308	0.228
tri_000_40964	Si ₂ Tb	3	-5.656	-5.681	-1.000e-06	0.00382	0.201	0.137
tri_000_40974	Se ₂ Tb	3	3.852	-5.093	-1.000e-06	0.00437	1.7	3.591
tri_000_40992	CoNd	2	-3.68	-5.452	-1.400e-05	0.00269	1.112	1.002
tri_000_40997	CaNYb	3	-4.553	-4.751	-4.000e-06	0.00553	0.468	0.583
tri_000_41018	IrNi	2	-6.952	-7.108	4.000e-06	0.00155	0.193	0.168
tri_000_41022	CdGdGe	3	-3.529	-3.745	-4.000e-06	0.00277	0.578	0.524
tri_000_41098	Se ₂ Tb	3	-5.121	-5.295	1.000e-06	0.00205	1.506	0.957
tri_000_41099	AlMn	2	-6.268	-6.395	-1.000e-06	0.00135	0.274	0.105
tri_000_41102	NiRe	2	-8.372	-8.872	-6.000e-06	0.00787	0.295	0.201
tri_000_41105	Bi ₂ Tb	3	-4.179	-4.44	-1.000e-06	0.00495	1.007	0.788
tri_000_41130	MoRu	2	-9.63	-9.997	-6.000e-06	0.00243	0.308	0.172
tri_000_41169	AsCoSiTb	4	-5.874	-5.953	-4.510e-04	0.00895	0.243	0.207
tri_000_41175	GdSSeV	4	-5.995	-6.395	1.000e-06	0.00142	0.224	0.514
tri_000_41199	DyEu	2	-3.041	-3.068	-9.700e-06	0.00399	0.179	0.128
tri_000_41207	Nd ₂	2	-4.649	-4.685	-1.380e-05	0.00059	0.223	0.223
tri_000_41216	BaDyGe	3	-3.423	-4.035	-1.000e-06	0.00633	0.546	0.347

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_41218	NiOs	2	-7.886	-8.193	-5.800e-05	0.00884	0.179	0.102
tri_000_41241	SnYb	2	-0.875	-3.134	-1.600e-06	0.00703	1.068	0.678
tri_000_41249	NiZn	2	-3.252	-3.44	-4.000e-05	0.00775	0.282	0.216
tri_000_41254	FeIr	2	-8.367	-8.518	-5.000e-06	0.00257	0.19	0.313
tri_000_41259	CLuMn	3	-7.381	-7.716	-1.000e-06	0.00419	0.681	0.85
tri_000_41291	Tb ₂	2	-4.54	-4.549	-2.400e-06	0.00352	0.107	0.13
tri_000_41307	PSiTb	3	-5.692	-5.75	-1.000e-06	0.00468	0.188	0.109
tri_000_41312	MnSn ₂	3	-4.848	-5.193	0.000e+00	0.00259	0.686	0.468
tri_000_41313	AsNTb	3	-5.818	-6.654	0.000e+00	0.00587	0.732	0.699
tri_000_41320	Ge ₂ Yb	3	-3.582	-3.951	1.000e-06	0.00538	0.461	0.31
tri_000_41329	GeYbZn	3	-2.906	-2.914	-1.900e-06	0.00175	0.109	0.162
tri_000_41356	Bi ₂ CoYb	4	-4.025	-4.28	-6.000e-06	0.00747	0.482	1.405
tri_000_41359	MnS ₂	3	-5.889	-6.055	-4.000e-06	0.0069	0.252	0.32
tri_000_41377	RuZr	2	-8.839	-8.963	-5.000e-06	0.00445	0.307	0.334
tri_000_41382	FeSiYb	3	-5.202	-5.217	-3.000e-06	0.00333	0.125	0.122
tri_000_41397	CaGd	2	-3.141	-3.146	-1.400e-06	0.00331	0.086	0.091
tri_000_41405	GdPPr	3	-5.613	-5.842	-3.000e-06	0.00859	0.383	0.241
tri_000_41422	Gd ₂ Se ₂	4	-5.62	-5.769	-6.000e-06	0.00303	0.318	0.262
tri_000_41432	GePdTb	3	-5.4	-5.726	-1.000e-06	0.0067	0.516	0.46
tri_000_41441	CoZr	2	-6.88	-7.805	-7.000e-06	0.00446	1.007	0.676
tri_000_41445	MnRe	2	-10.43	-10.603	-6.000e-06	0.0068	0.205	0.304
tri_000_41459	AlGdPd	3	-5.216	-5.278	-2.000e-06	0.00346	0.295	0.364
tri_000_41477	MnPt	2	-6.937	-7.448	0.000e+00	0.00462	0.483	0.314
tri_000_41500	CNd	2	-5.217	-6.37	-1.000e-06	0.00275	0.411	0.456
tri_000_41535	HMnTb	3	-5.121	-5.389	-1.220e-04	0.00388	0.263	0.496
tri_000_41555	CGaGd	3	-5.535	-5.707	0.000e+00	0.00718	0.274	0.267
tri_000_41562	AlNdP	3	-5.206	-5.342	0.000e+00	0.00258	0.268	0.173
tri_000_41581	DyRhYb	3	-4.822	-4.904	-3.000e-06	0.00295	0.267	0.36
tri_000_41592	DyTm	2	-4.452	-4.496	-1.200e-06	0.00481	0.157	0.17
tri_000_41656	NiOs	2	-8.113	-8.209	-1.500e-05	0.00515	0.131	0.11
tri_000_41678	NiZn	2	-3.346	-3.435	-2.400e-06	0.00537	0.237	0.246
tri_000_41688	ErRu	2	-5.96	-6.772	1.000e-06	0.00275	0.467	0.512
tri_000_41698	Ge ₂ Yb	3	-3.973	-4.059	-1.000e-05	0.00668	0.233	0.215
tri_000_41731	HDyOSr	4	-4.877	-5.037	0.000e+00	0.00695	0.23	0.368
tri_000_41742	NdY	2	-5.482	-5.545	-1.000e-06	0.00138	0.267	0.254
tri_000_41744	RuSiTbV	4	-6.633	-7.151	-3.300e-05	0.00569	1.103	0.762
tri_000_41745	CoZn	2	-3.901	-3.979	-5.700e-06	0.00575	0.191	0.169
tri_000_41746	GdPdSb ₂	4	-5.091	-5.201	-6.000e-06	0.00434	0.322	0.215
tri_000_41749	BiGdPdSb	4	-4.972	-5.032	-1.000e-06	0.00476	0.291	0.329
tri_000_41750	NdPSr	3	-4.445	-4.746	-9.000e-06	0.00452	0.99	1.088
tri_000_41764	B ₂ Ru	3	-7.262	-7.562	0.000e+00	0.00314	0.454	0.729
tri_000_41768	PdRu	2	-6.959	-6.989	3.000e-06	0.00181	0.064	0.038
tri_000_41800	Rh ₂ Yb ₂	4	-4.832	-4.97	3.000e-06	0.00085	0.371	0.256
tri_000_41885	PSiYb	3	-4.436	-4.62	-1.000e-06	0.0042	0.424	0.242
tri_000_41921	CdCoCr	3	-4.862	-5.314	-2.000e-05	0.00306	0.706	1.478
tri_000_41956	AlRu	2	-6.724	-6.95	-2.000e-06	0.00493	0.296	0.181
tri_000_41990	RhTb	2	-6.367	-6.672	0.000e+00	0.00176	0.636	0.593
tri_000_41993	PbYb	2	-2.868	-2.958	4.000e-07	0.00462	0.32	0.236
tri_000_42017	DyGeNi	3	-5.043	-5.595	2.000e-06	0.00631	0.806	0.783
tri_000_42018	Se ₂ Tb	3	-5.063	-5.251	-1.800e-05	0.00718	0.721	0.713
tri_000_42027	CuMn	2	-5.941	-6.03	0.000e+00	0.00857	0.166	0.097
tri_000_42028	AuNdP	3	-5.136	-5.411	-1.000e-06	0.00397	0.443	0.598

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_42082	MnPd	2	-6.77	-6.824	1.000e-06	0.00317	0.121	0.099
tri_000_42085	NiTi	2	-6.619	-6.739	1.300e-05	0.00705	0.226	0.124
tri_000_42122	FeIr	2	-7.894	-8.466	0.000e+00	0.0067	0.499	0.415
tri_000_42133	CrSeTb	3	-5.802	-6.029	3.000e-06	0.00445	0.203	0.299
tri_000_42141	CoRu	2	-7.809	-7.966	0.000e+00	0.00319	0.214	0.26
tri_000_42180	GeTbTe	3	-4.269	-4.723	-2.000e-06	0.00636	1.157	0.824
tri_000_42202	CNdZr	3	-7.52	-7.793	1.000e-06	0.00541	0.511	0.494
tri_000_42229	GdPPt	3	-5.984	-6.724	0.000e+00	0.00425	0.7	0.494
tri_000_42269	NiZn	2	-3.332	-3.428	-8.000e-07	0.00571	0.152	0.099
tri_000_42281	InRu	2	-5.074	-5.546	-4.000e-06	0.00937	0.425	0.211
tri_000_42291	PdYb	2	-3.877	-4.2	-7.000e-07	0.00158	0.874	0.724
tri_000_42297	Ni ₃	3	-5.387	-5.412	-2.000e-06	0.00726	0.109	0.114
tri_000_42311	DyMnSe	3	-5.714	-6.134	-4.000e-06	0.00765	0.747	0.614
tri_000_42321	H ₂ Mn	3	-3.665	-5.119	-2.800e-05	0.00402	0.301	0.553
tri_000_42336	FePd	2	-6.293	-6.332	3.000e-06	0.00473	0.133	0.162
tri_000_42374	S ₂ TiYb	4	-5.9	-6.006	4.000e-06	0.00421	0.198	0.108
tri_000_42375	GeYb	2	-0.791	-3.374	1.240e-05	0.00283	1.332	0.998
tri_000_42378	GdPb	2	-4.374	-4.428	-4.900e-06	0.00851	0.156	0.086
tri_000_42379	TbTl	2	-3.493	-3.614	-8.500e-05	0.0034	0.26	0.183
tri_000_42384	DyGaLa	3	-3.977	-4.373	-2.000e-06	0.006	0.694	0.56
tri_000_42389	MnSn	2	-4.826	-5.788	0.000e+00	0.00166	0.711	0.691
tri_000_42390	AlCo	2	-5.414	-5.705	-2.300e-05	0.00376	0.347	0.152
tri_000_42391	GeSbSeTb	4	-4.546	-5.007	-7.000e-06	0.00797	0.476	0.461
tri_000_42392	AlDySi	3	-4.947	-5.169	-4.000e-06	0.00853	0.193	0.508
tri_000_42403	DyTe	2	-5.007	-5.098	-4.000e-06	0.00566	0.216	0.128
tri_000_42436	SiThYb	3	-4.448	-4.86	0.000e+00	0.00605	0.618	0.594
tri_000_42458	CDyGe	3	-6.094	-6.069	1.000e-06	0.00684	0.41	0.342
tri_000_42496	BaSiYb	3	-2.415	-3.098	-1.500e-06	0.00334	0.702	0.519
tri_000_42504	DyLu	2	-4.477	-4.489	6.200e-06	0.00204	0.165	0.143
tri_000_42519	CGd	2	-5.75	-6.758	1.000e-06	0.0056	1.255	0.986
tri_000_42557	LaTb	2	-4.633	-4.678	-7.000e-06	0.00663	0.263	0.184
tri_000_42585	Ru ₂	2	-9.057	-9.24	-5.000e-06	0.00136	0.19	0.159
tri_000_42597	GaGdSi	3	-4.943	-4.963	0.000e+00	0.00278	0.085	0.061
tri_000_42624	Br ₂ Tb	3	-3.632	-4.238	-8.000e-06	0.00508	0.402	0.403
tri_000_42650	MnTi	2	-8.302	-8.457	-1.200e-05	0.00151	0.182	0.137
tri_000_42661	CBMn	3	-7.531	-8.279	0.000e+00	0.00367	0.587	0.644
tri_000_42663	LiNi	2	-3.468	-3.739	-3.000e-07	0.00335	0.378	0.573
tri_000_42675	IrMnOs	3	-9.345	-9.664	-1.000e-06	0.00321	0.277	0.342
tri_000_42677	HBeGeYb	4	-3.515	-3.547	0.000e+00	0.00383	0.162	0.119
tri_000_42707	AuNi	2	-4.077	-4.142	-1.000e-05	0.00304	0.152	0.134
tri_000_42714	NiRe	2	-8.617	-8.873	-1.030e-04	0.00221	0.198	0.193
tri_000_42722	GePrYb	3	-3.661	-3.886	0.000e+00	0.00549	0.526	2.07
tri_000_42763	Dy ₂	2	-4.508	-4.524	2.000e-07	0.00075	0.113	0.087
tri_000_42765	Al ₂ CoIr	4	-5.522	-6.032	-5.000e-06	0.0041	0.43	0.947
tri_000_42799	Be ₂ PRu	4	-5.165	-5.824	-1.000e-06	0.00297	0.692	0.736
tri_000_42829	AsCrGdMn	4	-6.258	-6.874	-1.000e-06	0.00899	1.275	1.197
tri_000_42834	GeTb	2	-4.897	-5.23	-1.000e-06	0.00328	0.773	0.738
tri_000_42860	H ₂ Co	3	-3.227	-4.485	1.000e-06	0.00381	0.398	0.519
tri_000_42878	MnTeYb	3	-4.234	-4.67	-1.190e-04	0.00807	1.069	1.107
tri_000_42931	NdTb	2	-4.601	-4.614	-3.200e-06	0.00198	0.126	0.113
tri_000_42937	Tb ₂	2	-4.548	-4.55	-8.200e-06	0.00176	0.049	0.052
tri_000_42954	AsDyPtTe	4	-5.007	-5.38	0.000e+00	0.00388	0.463	1.16

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_42962	MnNi	2	-7.084	-7.146	4.000e-06	0.00706	0.139	0.075
tri_000_42979	Se ₂ Tb	3	-4.775	-5.235	-1.000e-06	0.00399	0.962	1.013
tri_000_42980	CoSiTb	3	-6.22	-6.292	8.000e-06	0.00337	0.174	0.164
tri_000_42990	GdSeSi	3	-4.44	-5.029	-1.100e-05	0.00558	0.688	0.819
tri_000_43001	GaRu	2	-6.039	-6.276	-1.000e-06	0.00107	0.312	0.274
tri_000_43042	NdTe	2	-0.509	-5.33	-2.000e-06	0.00252	1.227	0.913
tri_000_43046	CoDySi ₂	4	-5.492	-6.104	1.000e-06	0.00588	1.003	0.84
tri_000_43080	MnMo	2	-9.364	-9.751	0.000e+00	0.00267	0.203	0.169
tri_000_43100	CuGdZn	3	-3.034	-3.444	5.000e-06	0.00298	0.655	0.838
tri_000_43104	CRuY	3	-7.244	-8.562	-2.000e-06	0.00715	0.544	0.549
tri_000_43108	PrYb	2	-2.978	-3.05	-1.320e-05	0.001	0.312	0.307
tri_000_43116	CoGa ₂ Tb	4	-4.471	-4.712	0.000e+00	0.00584	0.987	1.172
tri_000_43146	GdNiTb	3	-4.918	-5.023	-1.600e-05	0.00617	0.285	0.3
tri_000_43157	NdTh	2	-5.951	-6.005	1.400e-05	0.0032	0.262	0.319
tri_000_43158	MnOs	2	-9.713	-10.102	-1.000e-06	0.00564	0.238	0.304
tri_000_43219	MnZn	2	-4.622	-4.782	3.200e-06	0.00116	0.293	0.246
tri_000_43220	BrSYb	3	-2.744	-3.859	-3.000e-06	0.00404	0.969	1.013
tri_000_43228	LiRu	2	-5.148	-5.397	-1.000e-06	0.00842	0.326	0.277
tri_000_43234	PSrTb	3	-4.312	-4.716	1.000e-06	0.00594	0.836	1.343
tri_000_43250	DyPb	2	-4.359	-4.375	-8.000e-07	0.00324	0.116	0.114
tri_000_43253	GdTe	2	-5.079	-5.176	-4.000e-06	0.00206	0.27	0.324
tri_000_43275	RuZn	2	-4.892	-5.068	-3.000e-06	0.00589	0.481	0.384
tri_000_43293	Ge ₂ Ru	3	-4.438	-6.138	-3.000e-06	0.00194	0.379	1.811
tri_000_43297	AuFe	2	-4.834	-5.037	-2.000e-06	0.0045	0.3	0.148
tri_000_43299	CoDyI	3	-4.183	-4.528	1.000e-06	0.00411	1.299	0.905
tri_000_43303	NiReZn	3	-5.9	-6.272	1.000e-06	0.0042	0.484	0.632
tri_000_43309	NiPd	2	-5.101	-5.199	-1.000e-06	0.00488	0.292	0.312
tri_000_43366	RuW	2	-10.643	-10.908	-3.000e-06	0.00422	0.411	0.223
tri_000_43372	GdLu	2	-4.496	-4.507	-2.150e-05	0.00274	0.084	0.063
tri_000_43400	SeTb	2	-5.195	-5.371	0.000e+00	0.00225	0.296	0.102
tri_000_43424	CoRu	2	-7.519	-7.918	0.000e+00	0.00935	0.438	0.473
tri_000_43492	DyMnSe ₂	4	-5.654	-5.95	0.000e+00	0.00319	0.484	1.449
tri_000_43516	PdRu	2	-6.48	-6.991	-3.000e-06	0.00667	0.409	0.228
tri_000_43517	CoPdSbYb	4	-4.606	-4.764	-2.000e-06	0.00763	0.323	0.318
tri_000_43518	HMnNd	3	-2.918	-5.21	4.000e-06	0.00863	0.685	0.58
tri_000_43520	DyHo	2	-4.469	-4.515	2.000e-07	0.00014	0.216	0.198
tri_000_43549	AsCoTb	3	-5.791	-6.265	0.000e+00	0.00513	0.568	0.391
tri_000_43581	CoNdTe ₂	4	-5.021	-5.183	-1.000e-06	0.00461	0.395	0.395
tri_000_43586	HfMn	2	-8.603	-9.224	5.000e-06	0.00659	0.576	0.614
tri_000_43617	CdGeSTb	4	-4.075	-4.209	-1.000e-06	0.00596	0.283	0.277
tri_000_43629	RuZr	2	-8.793	-8.961	2.000e-06	0.00739	0.376	0.322
tri_000_43685	MnPt	2	-6.912	-7.437	-7.084e-03	0.00597	0.505	0.568
tri_000_43702	Sn ₂ Yb	3	-2.933	-3.492	-3.000e-06	0.00448	0.48	0.352
tri_000_43705	AuMnPt	3	-5.443	-5.885	-2.000e-06	0.00589	0.511	0.537
tri_000_43731	BeNdSi ₂	4	-4.633	-4.836	0.000e+00	0.00441	0.294	0.29
tri_000_43732	IrTbYb	3	-5.212	-5.421	-1.000e-06	0.00638	0.383	0.535
tri_000_43738	DySe	2	-4.283	-5.759	0.000e+00	0.00149	1.402	1.324
tri_000_43779	PtSbTb	3	-5.577	-5.982	-1.000e-06	0.00916	0.795	0.615
tri_000_43795	AsIrNd	3	-6.345	-6.99	-1.000e-06	0.00328	0.616	0.597
tri_000_43857	CoSiTb	3	-6.089	-6.29	-6.000e-06	0.00734	0.334	0.351
tri_000_43882	NiV	2	-7.094	-7.371	-6.000e-06	0.00461	0.417	0.361
tri_000_43910	DySb	2	-4.919	-5.225	-1.000e-05	0.00257	0.815	0.737

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_43914	PbYb	2	-2.88	-2.959	-7.400e-06	0.00703	0.242	0.292
tri_000_43916	CoTb	2	-4.665	-5.676	-7.000e-06	0.0086	0.845	1.041
tri_000_43941	CGdTe	3	-5.165	-5.6	-3.100e-05	0.00943	0.961	0.896
tri_000_43963	CoFe	2	-7.347	-7.488	-1.900e-05	0.00346	0.187	0.174
tri_000_44017	BrGdPdSe	4	-4.559	-4.857	-4.000e-06	0.00366	0.58	2.808
tri_000_44045	RuZn	2	-4.829	-5.085	-2.000e-06	0.00214	0.281	0.201
tri_000_44058	GdS ₂	3	-5.54	-5.85	-4.000e-06	0.00193	1.309	1.088
tri_000_44069	RuTh	2	-7.195	-8.199	-2.130e-04	0.00308	0.646	0.665
tri_000_44091	Ga ₂ Yb	3	-2.949	-2.981	6.000e-07	0.00631	0.216	0.336
tri_000_44104	GdSbSi	3	-4.544	-5.051	-2.000e-06	0.00246	1.071	0.408
tri_000_44110	RuSc	2	-7.468	-7.905	0.000e+00	0.0026	0.398	0.183
tri_000_44114	BeRuSi	3	-5.166	-6.266	0.000e+00	0.00351	0.635	0.489
tri_000_44115	GdIrTe	3	-5.471	-6.323	-3.000e-06	0.00152	1.035	0.818
tri_000_44122	MnZn	2	-4.689	-4.791	-2.500e-06	0.00547	0.206	0.16
tri_000_44130	I ₂ Nd	3	-3.661	-3.894	-1.000e-06	0.00265	0.632	0.471
tri_000_44134	BeMn	2	-6.165	-6.329	-2.000e-06	0.00489	0.179	0.052
tri_000_44160	NdTe ₂	3	-4.492	-4.724	-8.000e-06	0.00606	1.101	0.983
tri_000_44195	CaGd	2	-3.126	-3.145	-2.400e-06	0.00313	0.169	0.068
tri_000_44201	GdSi ₂	3	-5.127	-5.698	-2.000e-06	0.00445	0.463	0.58
tri_000_44204	BiNdPt ₂	4	-5.588	-5.922	-2.000e-06	0.00534	0.452	0.434
tri_000_44256	DyGd	2	-4.513	-4.546	-3.000e-07	0.00095	0.189	0.145
tri_000_44264	InMn	2	-4.259	-5.027	-1.000e-06	0.00539	0.529	0.388
tri_000_44289	CoMn	2	-7.589	-7.981	-7.000e-06	0.00122	0.358	0.485
tri_000_44323	HLaRu	3	-5.281	-5.834	0.000e+00	0.00313	0.382	0.49
tri_000_44331	AuGaNd	3	-4.007	-4.383	-6.000e-06	0.00449	0.6	0.579
tri_000_44345	GdSn	2	-4.682	-4.703	-7.400e-06	0.00983	0.083	0.098
tri_000_44360	PdS ₂ Tb	4	-5.492	-5.744	-2.000e-06	0.00368	0.546	2.059
tri_000_44363	CDyTe	3	-5.184	-5.585	0.000e+00	0.00613	0.816	0.799
tri_000_44377	GdTb	2	-4.522	-4.565	4.000e-07	0.00241	0.199	0.165
tri_000_44397	BeSiYb	3	-3.874	-3.891	-2.000e-06	0.00314	0.076	0.106
tri_000_44433	OsRhRu	3	-8.392	-9.157	-3.000e-06	0.00803	0.443	0.419
tri_000_44437	AlNdSb	3	-4.203	-4.7	-1.000e-06	0.00698	1.267	0.779
tri_000_44465	DyTb	2	-4.536	-4.538	-4.200e-06	0.00085	0.034	0.054
tri_000_44487	GdLiNPd	4	-5.481	-5.678	1.000e-06	0.00959	0.811	1.913
tri_000_44511	NdSn	2	-4.717	-4.941	-1.600e-06	0.00134	0.753	0.608
tri_000_44524	CoDyTe	3	-5.252	-5.583	-6.000e-06	0.00898	0.394	1.858
tri_000_44539	CoV	2	-7.929	-7.981	-4.000e-06	0.00185	0.152	0.202
tri_000_44546	DyGa ₂	3	-4.022	-4.089	-2.000e-06	0.00679	0.179	0.149
tri_000_44569	SeYb	2	-4.023	-4.398	0.000e+00	0.00152	0.361	0.354
tri_000_44593	Sb ₂ TbTi	4	-5.839	-5.885	-1.000e-06	0.00495	0.151	0.158
tri_000_44607	SbSnTb	3	-4.323	-4.652	-3.000e-06	0.004	1.099	2.581
tri_000_44614	LiNdS ₂	4	-5.121	-5.43	-2.000e-06	0.00634	0.473	0.513
tri_000_44654	GdMgSi	3	-3.862	-4.232	-3.000e-06	0.00359	0.796	0.567
tri_000_44659	CBMn	3	-7.831	-8.281	0.000e+00	0.00822	0.438	0.354
tri_000_44661	MnTm	2	-5.252	-6.015	1.300e-05	0.00681	0.723	0.598
tri_000_44668	CoRe	2	-9.274	-9.652	-3.000e-06	0.00479	0.238	0.186
tri_000_44715	NiSZr	3	-5.526	-6.749	-2.000e-06	0.00382	1.361	1.266
tri_000_44723	AuNdTe	3	-4.378	-4.646	-1.000e-06	0.00455	0.743	0.524
tri_000_44746	GeNd	2	-4.998	-5.051	-2.000e-06	0.00471	0.328	0.254
tri_000_44770	CaGd	2	-3.072	-3.147	-4.700e-06	0.00355	0.286	0.235
tri_000_44799	FeRh	2	-7.471	-7.618	-3.000e-06	0.00135	0.124	0.062
tri_000_44852	DyISb	3	-4.016	-4.159	0.000e+00	0.00574	0.549	0.482

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_44883	GeNd ₂	3	-4.747	-5.017	0.000e+00	0.00805	0.439	0.422
tri_000_44927	AuTb	2	-4.657	-4.659	-2.100e-06	0.00292	0.035	0.038
tri_000_44932	PtTbTe	3	-5.264	-5.609	0.000e+00	0.00798	0.805	0.847
tri_000_44949	MnTe ₂	3	-5.004	-5.043	-2.300e-05	0.00759	0.13	0.122
tri_000_44963	NdSbSn	3	-4.166	-4.693	-8.000e-06	0.00308	1.11	0.945
tri_000_44978	MnRu ₂	3	-8.663	-9.017	0.000e+00	0.00376	0.323	0.355
tri_000_44981	SbSiTb	3	-4.555	-5.089	0.000e+00	0.00331	0.844	0.953
tri_000_44995	NdSn	2	-4.576	-4.928	-2.060e-05	0.00564	0.684	2.088
tri_000_45007	NiTi	2	-6.603	-6.898	-6.000e-06	0.0013	0.689	0.605
tri_000_45052	DyNiSi	3	-5.925	-5.93	-1.430e-04	0.00388	0.038	0.049
tri_000_45072	PtTeYb	3	-4.205	-4.635	-7.000e-06	0.00621	0.759	0.661
tri_000_45090	GdSn	2	-4.549	-4.711	-4.600e-06	0.00748	0.267	0.125
tri_000_45095	DyPSb	3	-4.164	-5.294	0.000e+00	0.00891	0.902	0.679
tri_000_45121	NdTb	2	-4.606	-4.614	-4.400e-06	0.00284	0.085	0.102
tri_000_45133	CoV	2	-7.898	-7.987	-6.000e-06	0.00201	0.141	0.107
tri_000_45169	Co ₂	2	-6.786	-6.822	0.000e+00	0.00676	0.131	0.13
tri_000_45183	NdPb	2	-4.555	-4.49	5.600e-06	0.00254	0.212	0.26
tri_000_45184	DyLu	2	-4.446	-4.487	7.000e-07	0.00301	0.175	0.15
tri_000_45211	Ga ₂ Nd	3	-4.154	-4.2	-1.000e-06	0.00589	0.154	0.105
tri_000_45245	PdRu	2	-6.745	-6.991	-3.000e-06	0.00332	0.281	0.164
tri_000_45288	Ru ₂	2	-8.866	-9.26	-1.000e-06	0.00452	0.281	0.172
tri_000_45342	FeTb	2	-4.682	-5.833	3.000e-06	0.00228	0.874	0.74
tri_000_45355	GdTm	2	-4.486	-4.52	-3.300e-06	0.00103	0.167	0.189
tri_000_45399	PtRu	2	-6.926	-7.542	0.000e+00	0.00301	0.486	0.541
tri_000_45402	Ni ₂	2	-5.325	-5.385	-1.600e-05	0.009	0.184	0.173
tri_000_45403	RhSbYb	3	-4.759	-5.0	1.600e-05	0.00263	1.135	1.047
tri_000_45434	RuZn	2	-5.015	-5.078	0.000e+00	0.00427	0.172	0.229
tri_000_45444	TeYb	2	-3.573	-3.817	2.700e-06	0.00368	0.388	0.413
tri_000_45445	GaMg ₂ Ru	4	-3.717	-3.793	-8.000e-06	0.00934	0.256	0.38
tri_000_45453	CoP ₂ Ru	4	-7.094	-7.195	-2.000e-06	0.0084	0.149	0.212
tri_000_45487	CdMn	2	-3.834	-4.062	-3.930e-05	0.00594	0.294	0.234
tri_000_45491	CoNdTe	3	-5.147	-5.671	-1.000e-06	0.00895	0.877	0.639
tri_000_45503	PtSnTb ₂	4	-5.148	-5.224	-7.000e-06	0.00557	0.423	0.41
tri_000_45524	GdNd	2	-4.575	-4.63	1.280e-05	0.00283	0.189	0.125
tri_000_45554	AuGdS	3	-4.702	-5.139	-1.000e-06	0.00303	0.4	0.327
tri_000_45568	NiZn	2	-3.369	-3.433	-8.300e-06	0.0026	0.162	0.128
tri_000_45569	DyGe	2	-4.918	-5.155	-1.000e-06	0.00304	0.637	0.609
tri_000_45583	PrTb	2	-4.593	-4.619	-9.300e-06	0.00461	0.137	0.144
tri_000_45606	CoDy	2	-3.899	-5.572	-2.000e-06	0.00631	0.962	0.701
tri_000_45623	AcDy	2	-4.018	-4.204	-6.200e-06	0.00178	0.547	0.339
tri_000_45656	CLiRu	3	-5.675	-6.618	0.000e+00	0.00589	0.371	0.329
tri_000_45683	Si ₂ Yb	3	-4.414	-4.46	-2.400e-05	0.00709	0.111	0.066
tri_000_45708	CoNdTe	3	-5.082	-5.67	0.000e+00	0.00948	0.945	2.226
tri_000_45781	CTb	2	-6.125	-6.83	-2.000e-06	0.00402	0.628	2.294
tri_000_45783	DyTb	2	-4.516	-4.539	9.000e-07	0.00181	0.136	0.087
tri_000_45788	Co ₃ Dy	4	-5.773	-6.12	-1.530e-04	0.00985	0.821	1.523
tri_000_45790	B ₂ Ru	3	-7.07	-7.385	-1.000e-06	0.00601	0.168	0.093
tri_000_45794	MnRh	2	-7.642	-8.034	-1.800e-05	0.00196	0.515	0.323
tri_000_45799	AgMn	2	-4.854	-5.085	-2.400e-05	0.00734	0.505	0.499
tri_000_45838	AsFeTb	3	-5.887	-6.429	-1.600e-05	0.00655	0.578	0.776
tri_000_45840	CoCu	2	-5.011	-5.105	3.000e-06	0.00259	0.204	0.301
tri_000_45841	AgYbZn	3	-1.781	-1.965	-1.000e-07	0.00327	0.252	0.17

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_000_45852	AsGdSi	3	-5.244	-5.451	5.000e-06	0.00217	0.405	0.378
tri_000_45875	DyNd	2	-4.571	-4.594	1.700e-06	0.00304	0.168	0.089
tri_000_45884	NdTeTi	3	-5.12	-5.581	-3.100e-05	0.00596	0.443	0.374
tri_000_45905	PtSiTb	3	-6.082	-6.5	-1.000e-06	0.00379	0.477	0.415
tri_000_45957	AsGdTl	3	-5.925	-6.245	3.000e-06	0.0023	0.655	1.883
tri_000_45983	CdNdSi	3	-3.116	-4.066	4.000e-06	0.00729	0.065	0.904
tri_000_45984	RuZr ₂	3	-8.767	-8.928	-3.000e-06	0.00606	0.472	0.399
tri_000_45988	CoGdPd	3	-5.536	-5.97	2.000e-06	0.00901	0.509	0.72
tri_000_45997	NiOs	2	-7.996	-8.192	-1.910e-04	0.00575	0.177	0.135
tri_000_46020	DyGa ₂	3	-3.997	-4.091	0.0000e+00	0.00554	0.232	0.111
tri_000_46022	TbTl	2	-3.491	-3.613	-7.000e-07	0.00381	0.299	0.312
tri_000_46038	MnZn	2	-4.587	-4.797	-5.400e-06	0.00301	0.226	0.109
tri_000_46057	Ge ₂ SiTb	4	-4.107	-5.024	-2.700e-05	0.00649	0.926	0.423
tri_000_46060	CoOs	2	-8.81	-8.988	-7.000e-06	0.00365	0.16	0.116
tri_000_46065	CaYb	2	-1.669	-1.686	-1.090e-05	0.00326	0.155	0.252
tri_000_46080	AlYbZn	3	-2.123	-2.437	-1.100e-06	0.00388	0.726	0.871
tri_000_46092	CoIr	2	-7.596	-7.84	-1.000e-06	0.00609	0.282	0.25
tri_001_00011	AsCoDy	3	-5.869	-6.262	-2.000e-06	0.00452	0.285	1.696
tri_001_00073	MoRu	2	-9.644	-9.998	-3.000e-06	0.00325	0.261	0.31
tri_001_00081	Cl ₂ Gd	3	-4.609	-4.697	-4.000e-06	0.00453	0.313	0.316
tri_001_00084	GdNdSi	3	-4.616	-5.208	1.000e-06	0.00196	0.416	0.388
tri_001_00102	AsNdSbTb	4	-5.583	-5.705	1.000e-06	0.00198	0.355	0.339
tri_001_00103	CaTlYb	3	-1.998	-2.069	-2.700e-06	0.00528	0.285	0.292
tri_001_00109	AsIrTb	3	-6.559	-6.965	-2.000e-06	0.00474	0.669	0.675
tri_001_00165	NiTc	2	-7.576	-7.837	-1.000e-06	0.00534	0.231	0.137
tri_001_00177	Al ₃ Nd	4	-3.952	-4.198	1.000e-06	0.00328	0.968	1.679
tri_001_00199	NdNiZn	3	-2.355	-3.609	-2.300e-05	0.0091	1.274	0.89
tri_001_00262	EuNd	2	-3.161	-3.21	2.000e-07	0.00372	0.311	0.428
tri_001_00276	Br ₂ Yb	3	-3.575	-3.708	1.000e-06	0.00783	0.322	0.231
tri_001_00289	CoDySi	3	-6.11	-6.29	-2.280e-04	0.00678	0.245	0.196
tri_001_00333	GaPdYb	3	-3.733	-3.959	-2.000e-06	0.00846	0.606	0.546
tri_001_00334	MnSiTc	3	-8.142	-8.345	0.0000e+00	0.00952	0.339	0.324
tri_001_00337	MnRh	2	-7.875	-8.124	-1.500e-05	0.00767	0.275	0.281
tri_001_00380	MoRuW	3	-9.932	-10.896	1.000e-06	0.00485	0.282	0.436
tri_001_00456	BiPdRhYb	4	-4.703	-4.895	-2.000e-06	0.00372	0.443	0.307
tri_001_00458	Tb ₂	2	-4.5	-4.547	-7.000e-07	0.00337	0.23	0.193
tri_001_00510	Pt ₂ RuZn	4	-5.386	-5.761	-1.000e-06	0.00458	0.84	0.923
tri_001_00518	FePdTl	3	-6.911	-7.202	7.000e-06	0.00824	0.554	0.629
tri_001_00541	DyY	2	-5.466	-5.483	1.000e-06	0.00142	0.077	0.055
tri_001_00548	AsGeRu	3	-5.164	-6.17	-1.000e-06	0.00487	0.372	0.539
tri_001_00562	CoIr	2	-7.518	-7.848	0.0000e+00	0.004	0.217	0.205
tri_001_00564	Se ₂ Tb	3	-4.914	-5.219	-1.800e-05	0.0039	0.927	1.228
tri_001_00578	BiNd	2	-4.798	-5.052	-2.000e-06	0.00482	0.788	0.923
tri_001_00603	NdTb	2	-4.564	-4.613	-1.000e-07	0.00544	0.226	0.261
tri_001_00607	BrGdNi	3	-4.236	-4.474	4.000e-06	0.00935	0.778	0.945
tri_001_00615	GePtYb	3	-4.72	-4.99	3.000e-06	0.00579	0.779	0.956
tri_001_00617	DyLiNiSi	4	1.523	-4.649	0.0000e+00	0.00752	1.962	2.145
tri_001_00642	TbTh	2	-5.935	-5.95	0.0000e+00	0.00326	0.103	0.113
tri_001_00659	IrMn	2	-8.953	-9.049	-1.000e-05	0.00556	0.137	0.129
tri_001_00706	DyTe	2	-4.972	-5.1	2.000e-06	0.00424	0.222	0.244
tri_001_00707	DyS	2	-5.129	-5.892	1.000e-06	0.00275	0.475	0.207
tri_001_00721	CuGdS	3	-4.725	-5.043	1.000e-06	0.0041	0.571	0.671

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_001_00727	Co ₂	2	-6.784	-6.823	-5.000e-06	0.00351	0.079	0.078
tri_001_00731	EuYb	2	-1.624	-1.642	3.800e-06	0.00321	0.237	0.138
tri_001_00734	As ₂ TbTi	4	-5.434	-6.233	-1.000e-06	0.00531	1.08	1.109
tri_001_00789	FePt	2	-6.609	-6.963	0.000e+00	0.00407	0.492	0.482
tri_001_00808	FeIr	2	-8.15	-8.514	-1.500e-05	0.00565	0.346	0.398
tri_001_00820	PrRu	2	-6.189	-6.739	-3.000e-06	0.00504	0.845	0.766
tri_001_00826	HoTb	2	-4.511	-4.526	-6.000e-07	0.0035	0.103	0.093
tri_001_00836	SnYb	2	-2.98	-3.151	-3.000e-07	0.00348	0.507	0.405
tri_001_00908	CCuNd	3	-5.53	-5.705	-9.000e-06	0.00564	0.217	0.311
tri_001_00911	DySb	2	-4.901	-5.225	1.000e-06	0.00337	0.868	0.514
tri_001_00913	Nd ₂ O ₂	4	-7.08	-7.48	7.000e-06	0.00883	0.748	2.035
tri_001_00959	NdY	2	-5.442	-5.543	-1.000e-06	0.00384	0.343	0.326
tri_001_01056	GdTh	2	-5.919	-5.962	-4.000e-06	0.00574	0.219	0.13
tri_001_01073	GaGdGe	3	-4.182	-4.667	-3.000e-06	0.00196	0.572	2.081
tri_001_01097	InTb	2	-3.804	-3.837	-3.600e-06	0.00596	0.128	0.122
tri_001_01099	Ru ₂	2	-8.827	-9.264	-2.200e-05	0.00195	0.255	0.141
tri_001_01100	Cl ₂ Tb	3	-4.544	-4.681	-6.000e-06	0.00608	0.191	0.229
tri_001_01118	GdTb	2	-4.522	-4.561	-3.160e-05	0.0019	0.203	0.144
tri_001_01134	CoNiZn	3	-4.433	-4.479	-4.200e-05	0.00464	0.11	0.102
tri_001_01196	Cl ₂ Yb	3	-4.121	-4.204	0.000e+00	0.00282	0.423	0.441
tri_001_01212	DyZn ₂	3	-2.153	-2.431	9.000e-07	0.0037	0.668	1.604
tri_001_01218	DyPb	2	-4.359	-4.373	-6.300e-06	0.00525	0.126	0.082
tri_001_01237	PdThYb	3	-4.91	-5.064	0.000e+00	0.00678	0.983	0.922
tri_001_01265	Ni ₂	2	-5.339	-5.384	-2.700e-05	0.00918	0.136	0.176
tri_001_01276	DyPZn	3	-4.4	-4.483	0.000e+00	0.00186	0.255	1.637
tri_001_01287	PdS ₂ Tb	4	-5.162	-5.735	0.000e+00	0.00616	1.228	1.954
tri_001_01327	LiNd	2	-3.118	-3.155	-3.000e-07	0.00403	0.24	0.158
tri_001_01335	Se ₂ Tb	3	-4.667	-5.251	-5.000e-06	0.00423	0.592	0.778
tri_001_01337	Ru ₂	2	-8.936	-9.243	-2.000e-06	0.00393	0.237	0.288
tri_001_01341	GdPtSe	3	-5.247	-5.848	-1.000e-06	0.00326	0.928	2.316
tri_001_01342	CoMn	2	-7.857	-7.981	-1.000e-06	0.00275	0.172	0.185
tri_001_01345	RuZr	2	-8.808	-8.958	2.000e-06	0.00734	0.363	0.408
tri_001_01351	NdTe	2	-4.886	-5.304	-2.000e-06	0.00359	0.391	0.29
tri_001_01398	AsNdTb	3	-5.076	-5.488	0.000e+00	0.00564	0.464	0.688
tri_001_01407	BaSiYb	3	-2.525	-3.107	-2.100e-06	0.00393	0.528	0.39
tri_001_01408	DyS ₂	3	-5.188	-5.803	-5.000e-06	0.0074	1.344	1.422
tri_001_01418	NdPr	2	-4.652	-4.693	-8.900e-06	0.0054	0.235	0.15
tri_001_01422	Ni ₂	2	-5.336	-5.384	9.000e-06	0.00419	0.126	0.119
tri_001_01427	CdCo	2	-2.732	-3.339	-3.000e-07	0.00425	0.537	0.527
tri_001_01428	Al ₂ Dy	3	-4.213	-4.505	-6.000e-06	0.00452	0.542	0.393
tri_001_01455	RuSb	2	-6.43	-6.508	-5.000e-06	0.00291	0.242	0.156
tri_001_01460	GdGe ₂	3	-4.795	-5.065	-3.000e-06	0.00589	0.422	0.218
tri_001_01499	LuRu	2	-6.708	-6.92	-4.000e-06	0.00558	0.446	0.229
tri_001_01538	AlSiTb	3	-5.165	-5.191	1.000e-06	0.00253	0.129	0.089
tri_001_01540	CaDy	2	-3.026	-3.099	-8.000e-07	0.00244	0.316	0.237
tri_001_01558	RhSeYb	3	-4.651	-5.13	-7.000e-06	0.00408	0.706	0.794
tri_001_01580	MnRh	2	-7.974	-8.132	-1.300e-05	0.00459	0.2	0.26
tri_001_01606	GaNdZn	3	-3.394	-3.448	0.000e+00	0.00388	0.251	0.227
tri_001_01644	CoCu	2	-5.087	-5.109	0.000e+00	0.00722	0.1	0.062
tri_001_01647	Br ₂ Dy	3	-4.139	-4.214	-2.000e-06	0.00943	0.253	0.156
tri_001_01650	HfRu	2	-9.678	-9.768	-4.000e-06	0.00265	0.163	0.219
tri_001_01654	NiV	2	-7.17	-7.257	-1.000e-06	0.00894	0.132	0.134

Table S4. The profile of generated materials with Triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tri_001_01733	GaNi	2	-4.233	-4.472	-3.500e-06	0.00679	0.292	0.242
tri_001_01762	CoRh	2	-6.798	-6.961	-1.100e-05	0.00636	0.119	0.051
tri_001_01769	GdMg ₂	3	-1.705	-2.555	-1.600e-06	0.00195	1.564	1.166
tri_001_01779	AlDySi	3	-5.103	-5.165	-5.000e-06	0.00347	0.183	0.131
tri_001_01801	FeNi	2	-6.642	-6.658	-3.200e-05	0.0028	0.078	0.071
tri_001_01809	H ₂ Tb	3	-3.379	-4.45	0.000e+00	0.00147	0.546	0.668
tri_001_01815	RuSi	2	-7.712	-7.804	-1.000e-06	0.00258	0.162	0.14
tri_001_01819	GdPtSe	3	-5.521	-5.863	0.000e+00	0.00575	0.755	0.56
tri_001_01843	H ₂ Mn	3	-4.115	-5.131	-3.000e-06	0.0024	0.38	0.625
tri_001_01863	PdSbTb	3	-5.232	-5.63	0.000e+00	0.00315	0.514	0.719
tri_001_01878	Tb ₂	2	-4.498	-4.546	2.000e-07	0.00251	0.217	0.287
tri_001_01881	GdTb	2	-4.55	-4.561	2.600e-06	0.00345	0.129	0.122
tri_001_01896	CdYb	2	-1.276	-1.331	7.000e-07	0.00702	0.237	0.269
tri_001_01917	FeZn	2	-4.298	-4.41	-2.970e-05	0.00712	0.312	0.192
tri_001_01932	BiDyPt	3	-4.905	-5.587	-4.000e-06	0.00729	0.846	0.719
tri_001_01947	MnPt	2	-6.836	-7.443	0.000e+00	0.00859	0.541	0.269
tri_001_01951	NdSb ₂	3	-4.42	-4.995	-3.000e-06	0.0074	1.411	0.817
tri_001_01967	InMn	2	-4.292	-5.022	2.000e-06	0.003	0.568	0.553
tri_001_01973	CoHf	2	-7.285	-8.57	-1.000e-06	0.00358	0.778	0.689
tri_001_01977	NiSbYb	3	-4.001	-4.369	-2.900e-05	0.00589	0.575	0.585
tri_001_02002	GdSi ₂	3	12.596	-5.608	0.000e+00	0.00562	1.377	1.91
tri_001_02011	Mo ₂ Ni	3	-8.604	-9.07	-1.000e-06	0.0086	0.67	0.479
tri_001_02026	FeWZn	3	-6.809	-7.182	-2.000e-06	0.00432	0.43	0.514
tri_001_02041	CCoGd	3	-6.904	-7.015	-2.300e-05	0.00663	0.265	0.348
tri_001_02050	CoDyGe	3	-5.777	-5.933	-4.000e-06	0.0061	0.285	1.581
tri_001_02077	GdY	2	-5.462	-5.502	-2.300e-05	0.00299	0.213	0.184
tri_001_02088	OsRuW	3	-10.694	-11.0	-1.900e-05	0.00342	0.322	0.334
tri_001_02112	GeNdTi	3	-5.718	-5.982	-5.000e-06	0.00869	0.943	0.883
tri_001_02115	DyPtSi	3	-6.474	-6.503	0.000e+00	0.00611	0.26	0.282
tri_001_02126	ErTb	2	-4.493	-4.517	2.500e-06	0.00323	0.138	0.178
tri_001_02144	NdY	2	-5.495	-5.543	1.000e-06	0.00154	0.219	0.107
tri_001_02155	NdTe ₂ Tm	4	-5.148	-5.182	-3.000e-06	0.00341	0.202	0.157
tri_001_02164	DySn	2	-4.506	-4.673	-1.000e-06	0.00957	0.687	0.427
tri_001_02165	As ₂ CuNd	4	-4.776	-4.916	-3.200e-05	0.00508	0.225	0.229
tri_001_02167	AlRu	2	-6.826	-6.963	-4.000e-06	0.00424	0.152	0.174
tri_001_02170	MnMo	2	-9.393	-9.632	-2.240e-04	0.0042	0.273	0.321

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation

Index	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_00006	DyLaRu ₂ Sn ₂	6	-5.933	-6.238	-1.000e-06	0.00867	0.757	1.722
hon_000_00081	Co ₂ Fe ₂ Si ₂	6	-6.905	-7.131	-8.000e-05	0.0092	0.536	0.386
hon_000_00085	Rh ₂ Se ₄ Tb ₂	8	-4.993	-5.734	-3.000e-06	0.00487	1.229	2.999
hon_000_00092	Fe ₂ SiTi ₂ TmY	7	-6.608	-7.07	0.000e+00	0.00588	1.286	2.593
hon_000_00125	Co ₂ SbTm ₂	5	-5.547	-5.885	1.200e-05	0.00869	0.77	0.543
hon_000_00136	Co ₂ Cu ₂ Se ₄	8	-3.143	-4.41	7.000e-06	0.00982	0.996	0.588
hon_000_00163	Cl ₄ Dy ₂ Ir ₂	8	-4.499	-5.267	-2.000e-06	0.00923	1.769	2.611
hon_000_00171	Br ₂ Cl ₂ Dy ₂ Pt	7	-3.627	-4.599	-1.000e-06	0.00378	2.068	4.34
hon_000_00182	HoLi ₃ Ni ₃	7	-3.718	-3.864	-8.000e-06	0.00706	0.429	0.522
hon_000_00199	Cl ₄ Pd ₂ Tb ₂	8	-3.824	-4.791	0.000e+00	0.00501	1.425	3.055
hon_000_00214	Cs ₃ SbTiYb ₂	7	-1.781	-1.826	-4.500e-05	0.00293	0.126	2.357
hon_000_00223	Gd ₂ Mg ₂ Sn ₂	6	-3.445	-3.623	3.000e-06	0.00285	0.641	0.431
hon_000_00258	Dy ₂ La ₂ Sn ₂	6	-4.419	-4.902	-3.000e-06	0.00898	1.535	2.368
hon_000_00265	CdGd ₂ Ni ₂ Tl	6	-3.651	-4.144	-1.100e-05	0.00707	1.737	2.226
hon_000_00272	CaI ₃ PtRu ₂	7	-6.518	-6.634	-5.000e-06	0.00964	0.381	1.075
hon_000_00298	GeMn ₂ Pt ₃	6	-6.6	-6.789	-1.000e-05	0.00924	0.541	0.604
hon_000_00299	Cs ₃ Gd ₂	5	-1.622	-1.663	-1.470e-05	0.00274	1.195	1.208
hon_000_00313	Cl ₄ Gd ₂ Pd ₂	8	-3.897	-4.819	-7.000e-06	0.00562	2.236	3.209
hon_000_00321	Co ₂ Ga ₄	6	-4.049	-4.543	0.000e+00	0.00462	0.793	1.266
hon_000_00347	Na ₄ Yb ₂	6	-1.215	-1.282	2.400e-06	0.00445	0.677	1.685
hon_000_00391	Al ₂ Co ₂ NiTi	6	-5.909	-6.402	-2.400e-05	0.00751	0.198	2.036
hon_000_00395	Fe ₂ Ga ₄	6	-4.472	-4.567	-5.000e-06	0.00422	1.162	1.285
hon_000_00428	AuEr ₂ Fe ₂ Sn	6	-5.466	-5.673	-1.000e-05	0.00737	1.241	2.279
hon_000_00437	AgGaGeSbTeTiYb ₂	8	-2.948	-3.238	0.000e+00	0.00692	0.692	1.461
hon_000_00449	Co ₂ SiSmZn	5	-4.787	-5.164	-1.800e-05	0.00858	0.725	1.953
hon_000_00488	AuCdCsK ₂ Yb ₂	7	-1.422	-1.529	-9.000e-06	0.00614	1.397	0.968
hon_000_00497	HgRu ₂ SbYb ₂	6	-3.754	-4.421	-1.000e-06	0.00466	0.972	0.647
hon_000_00498	AlInLu ₂ Ru ₂	6	-5.457	-5.817	-1.000e-06	0.00711	0.503	1.9
hon_000_00505	Dy ₆	6	-4.443	-4.519	-3.000e-06	0.00253	0.379	0.452
hon_000_00561	Co ₂ Pr	3	-5.994	-6.256	0.000e+00	0.00184	0.289	0.187
hon_000_00565	Co ₃ CrSiSn	6	-6.289	-6.593	1.200e-05	0.00798	1.083	0.654
hon_000_00578	Ca ₂ CdSrYb ₂	6	-1.518	-1.582	-1.700e-06	0.00275	0.815	0.769
hon_000_00589	Dy ₅ Ga	6	-4.299	-4.339	0.000e+00	0.00336	0.242	0.136
hon_000_00605	Co ₂ CuH ₀ ₂ Pb	6	-5.112	-5.233	-1.900e-05	0.00783	0.888	2.108
hon_000_00639	Gd ₃ Te ₃	6	-4.626	-5.196	0.000e+00	0.00539	1.688	2.821
hon_000_00665	Fe ₂ Mn ₃ Pd	6	-7.86	-7.912	-3.300e-05	0.00621	0.097	0.827
hon_000_00669	Li ₃ Ni ₃	6	-3.627	-3.684	-3.000e-05	0.00409	0.262	2.309
hon_000_00692	Cd ₂ IrSnSrYb ₂	7	-2.578	-3.086	0.000e+00	0.0048	1.273	3.1
hon_000_00698	Gd ₂ LuNa ₃	6	-2.569	-2.664	-8.000e-06	0.00278	0.826	1.511
hon_000_00700	Fe ₃ Ge ₃	6	-5.549	-6.175	0.000e+00	0.00652	0.402	1.146
hon_000_00712	EuGaGd ₂ HgNa ₂	7	-2.302	-2.548	0.000e+00	0.00436	0.646	1.359
hon_000_00721	Cd ₂ Tb ₄	6	-3.267	-3.491	-4.000e-06	0.00316	1.114	1.996
hon_000_00725	CdMg ₂ Nd ₂ Sn	6	-2.825	-3.011	-5.000e-06	0.00607	0.575	0.242
hon_000_00739	CaLiMnRu ₂	5	-5.424	-5.893	4.000e-06	0.00767	0.53	0.548
hon_000_00762	Co ₂ CuGaPr ₂	6	-5.093	-5.222	-3.000e-06	0.00774	0.564	1.35
hon_000_00778	Al ₆ Mn ₂	8	-4.881	-5.012	0.000e+00	0.00631	0.721	0.639
hon_000_00798	Ga ₂ Gd ₃ Zr	6	-4.547	-4.976	2.000e-06	0.00539	1.116	1.053
hon_000_00837	Cd ₂ Tl ₂ Yb ₂	6	-1.541	-1.718	-7.000e-06	0.00484	0.769	1.391
hon_000_00853	AlCaRu ₂ Sn	5	-5.372	-5.67	-1.000e-06	0.00709	0.616	1.373
hon_000_00880	MgNd ₃ Sn ₂	6	-3.965	-4.369	0.000e+00	0.00335	1.252	1.879
hon_000_00886	CuGaHf ₂ Ni ₂	6	-6.373	-6.566	-3.000e-06	0.00711	0.446	1.014
hon_000_00888	Co ₂ CuEr ₂ Ge	6	-5.427	-5.594	1.000e-06	0.00926	0.557	1.176

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_00893	Ba ₂ Gd ₂ Na	5	-2.362	-2.559	-1.000e-06	0.00195	1.595	1.985
hon_000_00925	GaNd ₂ SbSnTl ₃	8	-3.018	-3.718	-3.000e-06	0.0048	1.189	2.021
hon_000_00943	Mg ₂ Nd ₂ SrTb	6	-2.955	-3.083	0.000e+00	0.00221	0.821	0.604
hon_000_00956	EuGd ₂ Mg ₂	5	-2.468	-2.804	-6.000e-06	0.00197	1.163	2.097
hon_000_00970	LiNi ₂ Sn ₂	5	-3.945	-4.232	-1.000e-06	0.00584	0.951	0.552
hon_000_00987	Sn ₃ SrTb ₂	6	-3.847	-4.295	-1.300e-05	0.00557	0.706	3.053
hon_000_01027	P ₂ S ₂ Tl ₂ Yb ₂	8	-3.306	-3.993	0.000e+00	0.00642	1.26	1.772
hon_000_01034	CePdRu ₂ Sn ₄	8	-5.432	-5.868	-2.000e-06	0.00609	1.04	1.117
hon_000_01043	Al ₂ Fe ₂ HoMn ₂	7	-6.222	-6.618	-1.200e-05	0.00732	0.871	1.529
hon_000_01053	Bi ₂ Dy ₂ In ₂	6	-4.134	-4.083	-1.000e-06	0.00454	1.445	1.838
hon_000_01077	Ga ₄ Ru ₂	6	-5.017	-5.107	-2.000e-06	0.00727	0.239	0.229
hon_000_01082	Ga ₂ Ni ₂ Si ₂	6	-4.33	-4.663	-2.000e-06	0.00585	0.958	2.067
hon_000_01083	Cl ₆ Dy ₂	8	-4.586	-4.808	1.000e-06	0.00487	0.654	0.572
hon_000_01090	BaDy ₅	6	-3.895	-3.935	0.000e+00	0.00466	0.296	1.319
hon_000_01099	AuCa ₂ Mn ₂ SiZr	7	-5.479	-5.656	-1.000e-06	0.01	1.291	1.514
hon_000_01107	Co ₃ LiSn ₂	6	-4.758	-5.104	-5.000e-06	0.00478	0.547	2.421
hon_000_01180	CeDy ₄ Ga	6	-4.465	-4.544	-3.400e-05	0.0062	0.494	0.544
hon_000_01203	AlAu ₂ Ni ₃	6	-4.46	-4.56	-8.200e-05	0.00744	0.468	1.009
hon_000_01210	Fe ₂ Ga ₄	6	-4.434	-4.577	-1.100e-05	0.00587	0.505	1.183
hon_000_01220	BaCd ₂ MgTb ₂	6	-2.125	-2.422	0.000e+00	0.00167	1.309	0.922
hon_000_01277	Ga ₄ Ru ₂	6	-5.055	-5.129	-1.000e-06	0.00638	0.154	0.975
hon_000_01283	Cl ₄ RuYb ₂	7	-3.311	-4.275	-3.000e-06	0.00592	1.964	1.543
hon_000_01287	Al ₂ Co ₂ SnTh	6	-5.439	-5.639	4.000e-06	0.00566	0.721	0.771
hon_000_01291	CaI ₂ Fe ₃ Na	7	-5.415	-5.83	-1.000e-06	0.00791	0.684	1.874
hon_000_01301	AlGeNi ₃ Si	6	-5.193	-5.327	1.200e-05	0.00687	0.165	0.977
hon_000_01328	Al ₄ PtRu ₂ Si	8	-5.326	-6.039	-3.000e-06	0.00479	0.931	0.816
hon_000_01342	Fe ₅ Sn	6	-7.12	-7.192	-1.000e-05	0.00574	0.205	0.183
hon_000_01352	Dy ₅ Sn	6	-4.599	-4.652	-1.000e-06	0.00481	0.804	1.473
hon_000_01368	Cs ₃ Gd ₂ KSb	7	-2.171	-2.228	1.000e-06	0.00661	0.492	1.51
hon_000_01381	Sn ₄ Yb ₂	6	-3.184	-3.456	-5.000e-06	0.00651	0.664	0.591
hon_000_01385	Li ₂ Nd ₂ Si ₂ Sn ₂	8	-3.856	-4.41	-1.000e-05	0.00526	1.162	1.517
hon_000_01401	HHfNi ₂ PtSn	6	-5.603	-6.052	-3.900e-05	0.00955	0.319	2.095
hon_000_01441	CdDy ₂ Ru ₂ Sb	6	-5.214	-5.66	-9.000e-06	0.00627	1.067	1.673
hon_000_01471	Fe ₂ La ₂ Te ₂	6	-5.385	-5.726	-1.000e-06	0.00893	1.345	1.117
hon_000_01486	Ni ₃ Si ₃	6	-5.608	-5.788	-8.200e-05	0.00837	0.246	0.156
hon_000_01513	GaLi ₂ Mn ₃	6	-5.233	-5.474	0.000e+00	0.00328	0.637	0.526
hon_000_01530	GaGd ₂ LiMg ₂	6	-2.711	-2.993	0.000e+00	0.00522	1.843	2.489
hon_000_01543	AlFe ₂ MgSi ₂	6	-5.188	-5.47	-1.000e-06	0.00448	0.897	0.778
hon_000_01550	AsCo ₂ GaLu	5	-5.01	-5.468	-2.200e-05	0.00887	0.773	1.162
hon_000_01578	Cs ₄ Yb ₂	6	-0.709	-0.837	-1.000e-07	0.00147	0.902	0.896
hon_000_01589	Br ₄ Gd ₂ IrPd	8	-4.032	-4.641	0.000e+00	0.00548	1.795	1.572
hon_000_01612	HfNpRu ₂ Si ₂	6	-8.542	-8.802	0.000e+00	0.00902	1.108	1.69
hon_000_01633	HfRu ₃ Sn ₂	6	-7.426	-7.613	-6.400e-05	0.00808	0.294	1.082
hon_000_01650	Fe ₂ Ga ₄	6	-4.35	-4.847	-4.000e-06	0.00803	0.958	2.042
hon_000_01651	LiNd ₃ Sn ₄	8	-3.753	-4.521	-1.000e-06	0.00517	0.933	1.199
hon_000_01661	Ca ₃ CdGd ₂	6	-2.547	-2.584	-2.000e-06	0.00174	0.288	0.309
hon_000_01678	Ga ₂ MgRu ₂ U	6	-6.014	-6.431	0.000e+00	0.00454	0.753	0.797
hon_000_01722	AuNi ₂ Sb	4	-4.258	-4.428	-3.000e-06	0.00697	0.27	1.469
hon_000_01724	AlLaLiRu ₂ Sc ₂	7	-5.785	-5.922	-4.000e-06	0.00479	0.285	1.069
hon_000_01751	Dy ₂ Sn ₅ Tl	8	-3.885	-4.183	-1.000e-06	0.00389	1.238	0.775
hon_000_01788	Fe ₃ Si ₄ Tl	8	-5.57	-6.104	-5.000e-06	0.00713	1.231	1.79
hon_000_01794	Ga ₄ Mn ₂	6	-4.634	-4.824	0.000e+00	0.00475	0.553	1.121

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_01800	Ga ₂ Ge ₃ Mn ₂ Tm	8	-4.92	-5.299	-2.000e-06	0.00772	0.744	0.723
hon_000_01821	AlFe ₂ MgOsTi	6	-6.557	-6.832	-2.100e-05	0.0089	0.633	1.188
hon_000_01844	AlCo ₂ OsU	5	-7.527	-8.218	0.000e+00	0.00669	0.825	0.892
hon_000_01848	BaCdSnSrYb ₂	6	-1.775	-2.17	-2.000e-06	0.00442	0.65	1.812
hon_000_01877	Pr ₂ Ru ₄	6	-7.345	-7.676	-1.000e-06	0.00303	0.702	0.622
hon_000_01948	Na ₂ Tb ₂ Y ₂	6	-3.777	-3.911	-4.000e-06	0.00214	0.421	0.256
hon_000_01984	Li ₄ Ni ₂ PtSn	8	-3.655	-3.733	-1.000e-06	0.0067	0.483	1.709
hon_000_02014	Ge ₂ MgMn ₃	6	-5.901	-6.052	-3.000e-06	0.00251	0.725	1.224
hon_000_02019	Sn ₄ Yb ₂	6	-3.162	-3.456	-4.000e-06	0.00814	0.895	1.502
hon_000_02024	AuCo ₅	6	-5.759	-5.96	4.000e-06	0.00582	0.29	0.237
hon_000_02056	Co ₄ Ho ₂	6	-6.027	-6.33	-1.530e-04	0.00947	0.628	0.632
hon_000_02071	Ga ₂ Ru ₃ Ti	6	-6.936	-7.112	-2.400e-05	0.00837	0.526	2.603
hon_000_02074	La ₃ Mn ₂ Pd ₂	7	-6.145	-6.365	-4.000e-06	0.00401	1.305	2.37
hon_000_02086	Sr ₂ Tb ₂ Tl ₂	6	-2.731	-2.967	3.000e-06	0.00785	1.362	2.537
hon_000_02089	CdGeLa ₃ Mn ₂	7	-4.786	-5.481	-1.000e-06	0.00948	0.812	1.48
hon_000_02148	Al ₂ PbRu ₃	6	-6.115	-6.383	3.000e-06	0.00722	0.639	0.784
hon_000_02154	Na ₄ Yb ₂	6	-1.198	-1.28	-9.300e-06	0.00483	0.627	0.555
hon_000_02183	Al ₂ AsFe ₂ Ti	6	-5.939	-6.172	-2.400e-05	0.00933	0.559	1.837
hon_000_02190	LiRu ₂ Zr ₃	6	-7.553	-7.779	-3.000e-06	0.00627	0.55	0.519
hon_000_02206	CaGaGd ₂ MgTl	6	-2.888	-3.198	-1.000e-06	0.00528	1.291	2.831
hon_000_02239	NiPt ₂ Ru ₂ Sn	6	-6.167	-6.563	4.000e-06	0.00688	0.505	0.446
hon_000_02243	Br ₂ IPdTb ₂	6	-3.348	-4.362	0.000e+00	0.00404	2.121	2.458
hon_000_02261	Cl ₄ Rh ₂ Tb ₂	8	-4.309	-4.949	-7.000e-06	0.00745	1.586	1.4
hon_000_02278	Nd ₂ Sn ₄	6	-4.311	-4.549	0.000e+00	0.00382	0.436	2.509
hon_000_02286	Co ₂ Ge ₃ W	6	-6.265	-6.627	0.000e+00	0.00652	0.498	1.199
hon_000_02294	Dy ₂ Na ₄	6	-2.005	-2.043	-4.000e-06	0.00424	0.321	0.2
hon_000_02341	Cs ₂ Nd ₂ PbTl	6	-2.341	-2.819	1.000e-06	0.00541	1.956	1.99
hon_000_02350	Cs ₄ Yb ₂	6	-0.739	-0.856	-6.000e-06	0.00131	0.841	1.881
hon_000_02389	CoGeMn ₂ MoSi	6	-7.602	-7.719	1.000e-06	0.00785	0.699	0.381
hon_000_02423	Ga ₄ Tb ₂	6	-3.354	-3.987	-1.000e-06	0.00453	1.523	1.307
hon_000_02448	Ru ₂ SiY ₃	6	-6.295	-7.296	1.500e-05	0.00983	0.826	0.538
hon_000_02454	EuSn ₂ Yb ₂ Zr	6	-3.347	-3.884	2.000e-06	0.00726	1.983	1.019
hon_000_02503	AgCuNi ₂ Pr ₂	6	-4.689	-4.701	-1.000e-06	0.00658	0.178	0.227
hon_000_02519	Ce ₂ Nd ₃ Tl	6	-4.441	-4.697	-1.100e-05	0.00789	0.699	2.208
hon_000_02535	AlGaGeMn ₂ Tc	6	-6.354	-6.503	-2.000e-06	0.00912	0.344	1.69
hon_000_02559	Fe ₂ Ga ₄	6	-4.347	-4.851	0.000e+00	0.00967	0.918	2.03
hon_000_02561	AlCuEr ₂ InLiNi ₂	8	-4.089	-4.212	-6.000e-06	0.00698	0.541	1.038
hon_000_02643	Al ₄ Fe ₂	6	-5.115	-5.375	0.000e+00	0.0054	0.953	1.181
hon_000_02646	CaDy ₂ Pt ₂ Sb	6	-5.162	-5.44	2.000e-06	0.00591	0.543	1.298
hon_000_02648	CrOs ₂ Ru ₃ Sn	7	-8.189	-8.791	-4.000e-06	0.00948	0.484	1.296
hon_000_02656	Cd ₂ Sr ₂ Tb ₂	6	-2.12	-2.331	0.000e+00	0.00305	1.992	1.915
hon_000_02666	Br ₂ Dy ₂ Se ₃	7	-4.263	-4.792	-2.000e-06	0.00499	1.251	2.054
hon_000_02682	Ru ₅ Zr	6	-8.715	-9.205	-1.300e-05	0.00497	0.771	0.894
hon_000_02714	Ir ₂ Sn ₄ Tb ₂	8	-5.229	-5.632	0.000e+00	0.00758	1.654	1.57
hon_000_02725	GaNi ₂ Y ₂ Zn	6	-4.975	-5.075	1.000e-06	0.00679	0.431	0.406
hon_000_02745	Au ₂ GeNd ₂ Pd ₂ Yb	8	-4.417	-4.715	0.000e+00	0.00292	0.998	2.282
hon_000_02750	ErIrNi ₃ Sn ₂	7	-5.521	-5.604	2.000e-06	0.00759	0.36	1.013
hon_000_02758	Sn ₄ Tb ₂	6	-4.365	-4.569	0.000e+00	0.00366	1.741	1.899
hon_000_02780	Ru ₂ TlTm ₂	5	-5.806	-6.093	-4.000e-06	0.00769	0.634	1.431
hon_000_02794	GaGd ₂ MgSn ₂	6	-3.75	-4.064	-2.000e-06	0.00935	1.621	3.084
hon_000_02810	Na ₂ Sr ₂ Yb ₂	6	-1.326	-1.417	1.400e-06	0.00387	1.047	2.006
hon_000_02812	Eu ₂ Hg ₂ Tb ₂	6	-2.167	-2.51	-3.000e-06	0.00702	1.291	1.646

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_02842	Fe ₂ Ga ₂ Tm ₂	6	-5.235	-5.431	-1.400e-05	0.00726	0.764	2.181
hon_000_02873	AlAuInLuRu ₂	6	-5.078	-5.517	-3.000e-06	0.00897	0.809	1.473
hon_000_02901	Ag ₂ MgSnTb ₂	6	-3.329	-3.568	-1.000e-06	0.00441	0.805	2.098
hon_000_02906	Cd ₂ NdRu ₂ Sn ₂	7	-4.123	-4.526	-2.000e-06	0.00671	1.046	0.814
hon_000_02919	Ni ₃ RhSnTi	6	-6.189	-6.225	3.000e-06	0.00599	0.07	0.869
hon_000_02971	Cl ₄ Gd ₂ Ir	7	-4.082	-4.988	-2.000e-06	0.0055	1.396	2.525
hon_000_02978	Al ₃ Mn ₂	5	-5.534	-5.842	-2.000e-06	0.00446	0.424	1.21
hon_000_03015	Au ₂ Cd ₂ Tb ₂	6	-2.953	-3.329	1.000e-06	0.00797	0.982	0.537
hon_000_03045	Fe ₃ Ge ₃	6	-5.996	-6.266	-4.000e-06	0.00809	0.303	1.184
hon_000_03055	Al ₂ Co ₂ PdSbSc	7	-5.348	-5.687	-1.600e-05	0.00445	0.892	1.296
hon_000_03096	Al ₅ Mn ₂ W	8	-5.758	-6.285	3.000e-06	0.0084	0.745	1.486
hon_000_03101	Ni ₃ Si ₂ V	6	-6.362	-6.388	-3.000e-06	0.00482	0.087	1.489
hon_000_03139	AgGaRu ₂ Yb ₂	6	-4.417	-4.64	-2.000e-06	0.00451	0.312	1.798
hon_000_03151	Au ₃ Co ₃	6	-4.597	-4.635	-1.500e-05	0.00895	0.114	0.839
hon_000_03159	Sn ₄ Yb ₂	6	-3.034	-3.422	3.000e-06	0.00617	0.994	1.378
hon_000_03170	Gd ₃ NdSiSn	6	-4.573	-5.036	0.000e+00	0.00393	0.938	1.015
hon_000_03177	Ni ₃ SiTbTi	6	-6.02	-6.26	0.000e+00	0.00509	0.556	1.284
hon_000_03179	AlMn ₂ OsSn	5	-6.679	-7.123	-1.000e-06	0.00559	0.786	0.467
hon_000_03192	HoIn ₂ Tb ₃	6	-4.059	-4.163	0.000e+00	0.00807	0.396	0.473
hon_000_03195	Co ₃ GaU ₂	6	-7.725	-7.841	-9.000e-06	0.00919	0.204	0.295
hon_000_03196	HoNd ₂ Sn ₃	6	-4.543	-4.832	-2.000e-05	0.00743	1.033	1.393
hon_000_03218	Br ₆ Nd ₂	8	-4.243	-4.313	-2.000e-05	0.00416	0.43	0.389
hon_000_03229	HoLiNd ₂ PbSn	6	-3.951	-4.312	-2.000e-06	0.00768	2.136	1.312
hon_000_03242	Dy ₅ Pb	6	-4.451	-4.505	0.000e+00	0.00686	0.202	1.197
hon_000_03265	HgMgNd ₂ Sn	5	-2.811	-3.225	-3.000e-06	0.00363	1.627	2.47
hon_000_03278	Cs ₃ Nd ₂ Pb	6	-2.1	-2.361	-3.000e-06	0.00549	1.571	3.744
hon_000_03283	Co ₂ FeGeSi ₂	6	-6.192	-6.493	-1.000e-05	0.00396	0.459	1.323
hon_000_03345	Co ₃ Ga ₃	6	-4.922	-5.016	0.000e+00	0.00768	0.161	0.19
hon_000_03373	Br ₄ Ir ₂ Nd ₂	8	-4.328	-4.91	0.000e+00	0.00513	1.599	3.11
hon_000_03376	As ₂ Cl ₄ Tb ₂	8	-3.089	-4.475	-3.000e-06	0.00531	1.444	2.161
hon_000_03417	Br ₄ Ir ₂ Nd ₂	8	-4.215	-4.982	-1.000e-06	0.00467	1.585	2.754
hon_000_03459	CdSr ₃ Yb ₂	6	-1.413	-1.475	-6.400e-06	0.00559	1.038	1.827
hon_000_03469	Ce ₂ CuFe ₂ Zn	6	-5.417	-5.607	2.000e-06	0.00762	0.383	1.036
hon_000_03479	AlNdNi ₂ Si	5	-5.165	-5.507	-2.400e-05	0.0082	1.22	1.072
hon_000_03512	Gd ₂ LuRu ₂ Zr	6	-6.366	-7.069	-1.000e-06	0.00561	0.512	0.942
hon_000_03536	Cs ₄ Yb ₂	6	-0.708	-0.838	-6.300e-06	0.00292	0.916	1.602
hon_000_03546	AuCa ₂ Co ₂ Ga	6	-4.005	-4.114	4.000e-06	0.00567	0.989	1.688
hon_000_03548	MgNd ₂ P ₂ Sn ₂	7	-4.28	-4.914	0.000e+00	0.00457	1.932	3.543
hon_000_03560	Cl ₃ Nd ₂ TeW	7	-4.739	-5.29	-2.000e-06	0.00416	1.178	3.047
hon_000_03561	Fe ₂ PtSi ₂	5	-6.476	-6.865	-1.000e-06	0.00894	0.939	2.373
hon_000_03629	Fe ₂ Pt ₄ Y	7	-6.482	-6.908	-5.000e-06	0.00899	0.853	1.283
hon_000_03669	MgSnTb ₂ Tl ₂	6	-3.233	-3.421	0.000e+00	0.00402	0.374	0.474
hon_000_03675	AlCo ₂ NiSi ₄	8	-5.481	-5.921	5.000e-06	0.00718	1.2	2.238
hon_000_03677	Na ₃ Yb ₃	6	-1.188	-1.302	6.000e-07	0.00623	0.593	2.624
hon_000_03687	Br ₄ Gd ₂ Sn	7	-2.939	-4.045	-1.000e-06	0.00283	2.044	1.455
hon_000_03731	CrGa ₂ GeNi ₂	6	-4.785	-5.12	-9.000e-06	0.00687	0.523	0.44
hon_000_03741	AlCo ₂ Nd	4	-5.122	-5.842	-4.000e-06	0.00429	0.741	0.836
hon_000_03745	Fe ₂ PdZr ₃	6	-7.689	-8.013	-1.000e-06	0.00295	0.891	1.839
hon_000_03754	PdRu ₂ SnU	5	-7.46	-7.997	-4.000e-06	0.00806	0.297	2.099
hon_000_03797	Fe ₂ Ga ₂ SiY	6	-5.262	-5.949	-8.000e-06	0.00595	0.623	1.972
hon_000_03822	AlGa ₂ Ni ₃	6	-4.503	-4.663	1.300e-05	0.00545	0.369	0.95
hon_000_03833	Al ₅ Ru ₂	7	-4.865	-5.459	0.000e+00	0.00488	0.676	0.648

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_03855	PRu ₂ ScSi	5	-7.154	-7.604	-1.000e-06	0.0064	0.806	0.493
hon_000_03871	AlCo ₂ Ge ₂ Nd	6	-5.417	-5.641	-4.100e-05	0.0077	0.59	1.897
hon_000_03879	GeMn ₂ SbTe ₃	7	-4.612	-5.092	1.300e-05	0.00397	1.135	3.802
hon_000_03892	AuCo ₂ Sn ₃	6	-4.39	-4.627	4.000e-06	0.00746	1.032	1.026
hon_000_03936	Li ₃ Ru ₂	5	-4.24	-4.577	-2.000e-06	0.00995	0.651	1.823
hon_000_03937	Cs ₃ Gd ₂ Sn	6	-2.027	-2.367	3.000e-06	0.00586	1.424	3.089
hon_000_03997	CaCdTl ₂ Yb ₂	6	-1.813	-2.122	-3.000e-06	0.00482	1.639	3.111
hon_000_04001	Co ₃ Ga ₃	6	-4.977	-5.029	-2.000e-06	0.00724	0.383	1.08
hon_000_04017	Co ₃ Mn ₂ Si	6	-7.152	-7.523	2.000e-06	0.00596	0.459	1.219
hon_000_04029	CeSnTb ₃ Zr	6	-5.294	-5.485	-4.000e-06	0.00372	0.421	0.374
hon_000_04032	AlFe ₂ GaLiPd	6	-5.087	-5.185	-4.000e-06	0.00439	0.291	1.132
hon_000_04044	BrI ₃ Ir ₂ Nd ₂	8	-4.223	-4.798	-1.000e-06	0.00705	1.718	2.739
hon_000_04060	Tb ₂ Tl ₄	6	-2.824	-3.171	0.000e+00	0.00387	1.265	2.536
hon_000_04099	GaGd ₃ MgZr	6	-4.243	-4.593	-3.000e-05	0.0051	1.19	2.074
hon_000_04102	Br ₄ OsYb ₂	7	-3.224	-3.874	-1.000e-06	0.00718	2.007	1.808
hon_000_04116	Nd ₂ Sn ₂ Tb ₂	6	-4.555	-4.832	-1.000e-06	0.00378	1.524	1.554
hon_000_04129	Nd ₂ Sn ₄	6	-4.364	-4.686	-7.000e-06	0.00494	1.447	3.265
hon_000_04133	Cs ₄ Yb ₂	6	-0.728	-0.856	6.000e-07	0.00145	0.912	1.893
hon_000_04162	AuCo ₄ Rh	6	-5.87	-6.028	-1.140e-04	0.00886	0.276	0.245
hon_000_04180	Ge ₂ Mn ₂ Ru ₂	6	-7.145	-7.444	-6.000e-06	0.00866	0.499	0.347
hon_000_04186	GaMn ₂ NiSi ₄	8	-5.766	-5.994	-4.100e-05	0.00543	0.214	0.796
hon_000_04200	Al ₂ CoFe ₂ Ge	6	-5.569	-5.951	-6.000e-06	0.00705	0.612	1.202
hon_000_04219	Al ₂ Mn ₃	5	-6.285	-6.782	-2.000e-06	0.00554	0.583	1.453
hon_000_04231	AlSn ₂ Tb ₃	6	-4.364	-4.558	-1.000e-06	0.00801	0.399	0.438
hon_000_04256	Dy ₃ Tl ₃	6	-3.335	-3.654	-1.000e-06	0.0047	1.36	0.749
hon_000_04265	Br ₆ Tb ₂	8	-4.22	-4.287	0.000e+00	0.00311	0.44	1.196
hon_000_04284	AlCo ₂ LiSb	5	-4.549	-4.716	6.000e-06	0.0084	0.343	1.79
hon_000_04289	Br ₄ Nd ₂ Ru	7	-3.715	-4.815	-3.000e-06	0.00581	1.667	2.533
hon_000_04303	Cd ₂ Pr ₂ Tb ₂	6	-3.187	-3.45	2.300e-05	0.00938	1.186	1.923
hon_000_04324	Co ₂ DyGaSb	5	-5.063	-5.449	-7.000e-06	0.005	1.086	1.102
hon_000_04342	AlFe ₂ PdSb ₂ Y	7	-5.722	-5.941	-2.300e-05	0.00656	0.658	0.703
hon_000_04343	Fe ₃ GaV ₂	6	-7.519	-7.58	0.000e+00	0.00822	0.282	1.336
hon_000_04398	Mn ₂ Mo ₂ Si ₂	6	-8.291	-8.521	-1.000e-06	0.00608	0.146	0.34
hon_000_04426	Al ₃ Ni ₃	6	-5.035	-5.094	-1.900e-05	0.00735	0.128	0.855
hon_000_04442	Ge ₃ Ru ₂ Si	6	-5.928	-6.259	3.000e-06	0.00772	0.647	1.003
hon_000_04473	Mn ₂ PrSbTi	5	-4.763	-6.884	-1.000e-06	0.00534	0.786	1.414
hon_000_04478	CuFe ₂ Li ₂ Sb	6	-3.879	-4.537	-4.000e-06	0.00462	0.854	0.768
hon_000_04503	Mn ₄ Si ₂	6	-7.523	-7.934	-1.500e-05	0.00361	0.651	1.463
hon_000_04506	Fe ₄ NbSi ₃	8	-7.196	-7.482	3.000e-06	0.00887	0.825	1.693
hon_000_04523	Gd ₂ SnThZr ₂	6	-6.152	-6.317	0.000e+00	0.00445	0.337	1.243
hon_000_04555	Cl ₄ Gd ₂ W	7	-4.201	-5.158	-1.000e-06	0.00423	1.967	2.055
hon_000_04582	AlCo ₄ Mn ₂	7	-6.991	-7.024	-5.600e-05	0.00943	0.066	0.697
hon_000_04619	Cr ₃ GaMn ₂	6	-8.025	-8.231	-1.000e-06	0.00835	0.587	1.164
hon_000_04669	Ag ₂ Dy ₂ Ga ₃	7	-3.356	-3.62	-2.000e-06	0.00416	0.627	1.532
hon_000_04676	Al ₃ Fe ₂ Sb	6	-4.851	-5.364	1.000e-06	0.00683	0.765	1.211
hon_000_04691	Al ₄ Gd ₃ Na	8	-3.593	-3.843	0.000e+00	0.0027	0.786	0.412
hon_000_04796	AlAuIrRu ₂ Sc	6	-6.687	-7.053	-2.000e-06	0.0047	0.622	1.388
hon_000_04797	GaMn ₂ PdU ₂	6	-7.816	-8.182	-2.000e-06	0.00371	0.394	0.418
hon_000_04808	LuPt ₂ Ru ₂	5	-6.952	-7.348	6.000e-06	0.00369	0.332	0.273
hon_000_04848	BaCd ₂ SrYb ₂	6	-1.358	-1.527	6.000e-07	0.00296	0.846	2.022
hon_000_04865	AlMgNdRu ₂ Si ₃	8	-5.66	-5.952	-2.000e-06	0.00815	0.951	2.021
hon_000_04878	FeGd ₂ K ₂ S ₂ Si	8	-3.983	-4.725	-6.000e-06	0.00483	1.354	2.415

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_04885	Dy ₂ Na ₄ Pt	7	-2.788	-2.873	-6.000e-06	0.00837	0.404	1.186
hon_000_04892	Co ₂ PtSiZr ₂	6	-7.144	-7.716	-1.100e-05	0.0088	1.321	2.34
hon_000_04922	Nd ₂ Sn ₂ Zr ₂	6	-5.504	-6.077	-1.000e-06	0.00635	0.784	1.546
hon_000_04928	Na ₂ SnTb ₂ Tl	6	-2.659	-3.187	-1.000e-06	0.00655	2.073	3.399
hon_000_04933	Ga ₄ Ni ₂	6	-3.546	-3.913	1.000e-06	0.0064	0.793	1.038
hon_000_04946	Co ₃ Li ₂ Mg ₂ Si	8	-3.952	-4.16	-2.800e-05	0.00899	0.548	0.414
hon_000_04985	AlCo ₂ LaSi	5	-5.449	-5.601	-2.000e-06	0.0075	0.388	1.687
hon_000_04996	AlCo ₂ GeV	5	-5.97	-6.253	-1.000e-06	0.00599	0.492	1.13
hon_000_05023	Cl ₄ Dy ₂ Ru	7	-3.962	-5.069	4.000e-06	0.0073	1.066	3.45
hon_000_05026	CuLi ₂ Ru ₃	6	-5.366	-5.649	-1.000e-06	0.00782	0.332	1.955
hon_000_05038	Gd ₂ MgSn ₃	6	-3.773	-4.247	6.000e-06	0.00386	1.602	2.209
hon_000_05053	Mn ₂ PrPt ₅	8	-6.227	-6.917	-7.000e-06	0.0039	0.577	1.161
hon_000_05105	AlCo ₂ Dy ₂ Si	6	-5.55	-5.701	-6.000e-06	0.00469	0.478	1.015
hon_000_05131	Li ₄ Ru ₂	6	-4.127	-4.216	3.000e-06	0.00557	0.225	2.43
hon_000_05146	AlGaHoNi ₂	5	-4.477	-4.945	-2.140e-04	0.00924	1.012	2.484
hon_000_05160	BiNi ₂ Tm ₂	5	-4.866	-5.252	2.000e-06	0.00604	0.791	1.561
hon_000_05164	AuCe ₂ Ni ₂ Zn	6	-4.876	-4.932	-1.000e-06	0.00596	0.438	1.088
hon_000_05176	Gd ₂ MgSn ₃	6	-3.702	-4.262	-3.000e-06	0.00682	1.598	1.557
hon_000_05201	Dy ₂ Ni ₂ SiZn	6	-4.775	-4.904	-1.030e-04	0.00581	0.394	1.048
hon_000_05226	Al ₃ Dy ₃	6	-4.314	-4.443	0.000e+00	0.00234	0.26	0.339
hon_000_05234	GaRu ₂ Tm ₂	5	-5.413	-6.447	0.000e+00	0.00469	1.707	1.785
hon_000_05254	Al ₂ MnNi ₃	6	-5.42	-5.735	-8.200e-05	0.00553	0.81	1.371
hon_000_05255	AuCa ₂ Fe ₂ Zn	6	-3.827	-4.084	-1.100e-05	0.00537	1.427	2.104
hon_000_05334	MgNa ₂ SnYb ₂	6	-1.75	-1.924	0.000e+00	0.00336	1.186	2.815
hon_000_05342	Co ₂ LiPTi ₂	6	-6.308	-6.494	-6.000e-06	0.00668	0.429	0.422
hon_000_05351	AcCaTl ₂ Yb ₂	6	-2.237	-2.452	0.000e+00	0.00322	1.984	2.632
hon_000_05389	KNa ₃ Tb ₂	6	-1.792	-2.037	-2.000e-06	0.00456	2.377	3.448
hon_000_05392	Al ₂ Ru ₂ Sc ₂	6	-6.492	-6.668	-2.000e-06	0.00306	0.399	1.199
hon_000_05393	ISnSrTeYb ₂	6	-2.656	-3.106	0.000e+00	0.0028	1.333	1.749
hon_000_05418	Co ₂ Pd ₂ Sb	5	-5.396	-5.65	-5.000e-06	0.00521	0.425	1.305
hon_000_05419	Sn ₃ Yb ₃	6	-2.925	-3.322	0.000e+00	0.00417	1.593	1.364
hon_000_05496	Sn ₂ Yb ₃	5	-2.477	-3.03	-5.000e-06	0.00533	1.832	1.04
hon_000_05521	CaPbSrTb ₂	5	-3.015	-3.149	0.000e+00	0.0052	0.513	2.839
hon_000_05554	NaPbSn ₂ Yb ₂	6	-2.735	-2.916	3.000e-06	0.00863	0.639	0.241
hon_000_05589	Ga ₂ Ni ₂ Zr ₂	6	-5.841	-6.022	0.000e+00	0.00476	0.813	1.346
hon_000_05608	AlCoMgNi ₃	6	-4.798	-4.909	-1.100e-05	0.00703	0.279	0.914
hon_000_05616	Ga ₃ Mn ₃	6	-5.582	-5.88	-3.000e-06	0.006	1.132	1.388
hon_000_05637	Co ₃ GeNi ₂	6	-5.813	-6.008	-4.000e-06	0.00825	0.225	0.865
hon_000_05640	AlAu ₂ Dy ₂ Ga ₂ Th	8	-4.248	-4.591	-2.000e-06	0.00642	0.998	0.694
hon_000_05654	GdMn ₂ PdSnY	6	-5.854	-6.314	-2.000e-06	0.00813	1.459	1.886
hon_000_05658	GaRu ₃ U ₂	6	-8.672	-8.973	1.000e-06	0.00573	0.466	1.171
hon_000_05661	CoGa ₃ Ni ₂	6	-4.405	-4.64	-1.000e-06	0.00355	0.814	1.824
hon_000_05670	GaRu ₃ Y ₂	6	-7.178	-7.459	-1.300e-05	0.00591	0.415	0.249
hon_000_05693	Gd ₂ Sn ₂ Zr ₂	6	-5.564	-6.031	-1.000e-06	0.005	0.603	0.488
hon_000_05698	CaCd ₃ Nd ₂	6	-2.2	-2.475	1.000e-06	0.00388	0.672	2.63
hon_000_05701	CdGaGd ₄	6	-3.672	-3.942	-4.000e-06	0.00172	1.051	1.747
hon_000_05729	AgCl ₄ Gd ₂ Mo	8	-3.87	-4.65	-2.000e-06	0.00449	1.33	1.991
hon_000_05768	AcCdNd ₂ Sr	5	-2.733	-3.118	-4.600e-05	0.00454	1.874	2.383
hon_000_05774	Al ₂ AuNi ₂	5	-4.468	-4.627	-1.000e-06	0.00631	0.322	0.339
hon_000_05790	Cl ₄ Tb ₂	6	-3.27	-4.571	-2.000e-06	0.00452	2.576	1.736
hon_000_05796	Ga ₃ Nd ₂ SrTlYb	8	-3.107	-3.276	0.000e+00	0.00868	0.626	0.398
hon_000_05806	Li ₂ Mn ₂ SbSn ₂	7	-4.447	-4.705	1.000e-06	0.00515	0.634	1.65

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_05868	AuFe ₂ Mg ₂ Tl	6	-3.541	-3.951	-5.000e-06	0.00829	0.947	2.022
hon_000_05892	Sn ₃ SrYb ₂	6	-2.861	-3.265	-2.000e-06	0.00267	0.877	3.642
hon_000_05912	Ni ₂ Si ₂ Te	5	-4.726	-4.98	0.000e+00	0.00735	0.513	1.121
hon_000_05927	Br ₄ Gd ₂ Pd	7	-3.331	-4.154	-3.000e-05	0.00477	1.042	1.13
hon_000_05944	Ga ₂ LiMg ₂ Ni ₂	7	-3.044	-3.276	0.000e+00	0.00478	1.05	2.149
hon_000_05966	CaGd ₂ LiMg ₂	6	-2.51	-2.626	1.000e-06	0.00239	0.985	2.082
hon_000_05986	Dy ₅ Mg	6	-3.959	-3.995	-1.000e-06	0.00365	0.252	1.177
hon_000_06020	PdSe ₃ TlYb ₂	7	-3.494	-4.178	0.000e+00	0.00673	1.749	3.091
hon_000_06065	Au ₂ GaRu ₂ U	6	-5.958	-6.612	1.000e-06	0.00952	0.429	1.551
hon_000_06066	CdNd ₂ SbSr	5	-3.119	-3.687	-8.000e-06	0.00418	1.469	1.247
hon_000_06078	Al ₃ Ni ₂ Ru	6	-5.46	-5.741	-2.000e-06	0.00549	0.526	1.886
hon_000_06090	Rb ₂ SbSnYb ₂	6	-1.968	-2.515	-1.000e-05	0.00475	1.299	2.247
hon_000_06092	DyMgTb ₄	6	-3.978	-4.016	0.000e+00	0.0042	0.251	0.291
hon_000_06103	Cr ₃ Ni ₂ Os	6	-8.306	-8.357	-1.000e-06	0.00404	0.131	0.074
hon_000_06112	Co ₂ ErZn ₂	5	-3.74	-4.228	0.000e+00	0.00555	0.729	1.685
hon_000_06113	Al ₂ Tb ₂ Zn ₂	6	-2.869	-3.575	-1.000e-06	0.00353	2.014	1.461
hon_000_06114	Au ₂ Cl ₄ Nd ₂	8	-3.216	-4.339	-1.000e-06	0.00503	1.645	2.761
hon_000_06121	CeCoFe ₂ Ga ₃	7	-5.36	-5.506	8.000e-06	0.00723	0.22	2.043
hon_000_06152	Al ₂ CuFe ₂ Li	6	-4.699	-4.994	-1.500e-05	0.00731	0.344	0.345
hon_000_06158	Ag ₂ Dy ₂ Pb ₂	6	-3.653	-3.728	2.000e-06	0.00341	0.668	1.232
hon_000_06186	Co ₂ La	3	-6.109	-6.331	0.000e+00	0.00444	0.307	0.304
hon_000_06189	Fe ₂ Ga ₃ Si	6	-4.793	-5.063	-2.000e-06	0.00535	0.964	1.59
hon_000_06191	AlCuNi ₂ Sc ₂	6	-5.339	-5.492	-6.000e-06	0.00607	0.459	1.226
hon_000_06196	CoGeNa ₃ Yb ₂	7	-2.361	-2.566	-1.000e-06	0.00396	2.004	2.253
hon_000_06205	CoFe ₂ Ga ₃	6	-5.218	-5.339	-1.700e-05	0.00834	0.809	1.955
hon_000_06227	Sn ₄ Yb ₂	6	-3.184	-3.455	-2.000e-06	0.00657	0.881	0.452
hon_000_06266	I ₄ PdTb ₂	7	-3.019	-4.011	0.000e+00	0.00791	2.022	3.039
hon_000_06286	CaGd ₂ LaMg	5	-3.044	-3.274	-6.000e-06	0.00287	1.311	2.01
hon_000_06290	Cs ₃ Dy ₂ Tl	6	-1.699	-1.934	-3.000e-06	0.00372	1.319	2.232
hon_000_06299	Dy ₂ In ₂ Pd ₂	6	-4.887	-4.66	0.000e+00	0.00193	0.368	1.258
hon_000_06317	BaSnTlYb ₂	5	-2.243	-2.647	0.000e+00	0.00313	1.182	1.107
hon_000_06343	Al ₂ Ni ₂ Si ₂	6	-4.818	-5.171	6.000e-06	0.0069	0.836	2.14
hon_000_06387	Al ₃ InRu ₂	6	-5.211	-5.714	-3.000e-06	0.00841	0.503	1.702
hon_000_06396	Ga ₄ Ni ₂	6	-3.717	-3.856	0.000e+00	0.00703	0.573	1.787
hon_000_06400	CaDy ₄ Mg	6	-3.43	-3.507	0.000e+00	0.00274	0.864	1.731
hon_000_06402	PdRu ₃ ScZr	6	-7.994	-8.151	-3.000e-06	0.00319	0.266	1.074
hon_000_06411	NbNi ₄ Si	6	-6.454	-6.569	1.000e-06	0.00837	0.274	0.314
hon_000_06421	Cs ₄ Yb ₂	6	-0.692	-0.837	-1.000e-07	0.00153	0.981	1.574
hon_000_06430	Gd ₂ Sn ₄	6	-4.457	-4.551	-1.000e-06	0.00528	0.385	0.263
hon_000_06432	GeMn ₂ NiSnTi ₃	8	-6.806	-7.015	-3.300e-05	0.00635	0.561	1.491
hon_000_06469	Gd ₂ MgSn ₃	6	-3.903	-4.214	1.000e-06	0.0042	1.63	1.565
hon_000_06475	Dy ₂ Te ₂	4	-3.485	-5.136	-1.100e-05	0.00742	2.525	2.983
hon_000_06526	Sn ₂ Tb ₂ Yb ₂	6	-3.293	-3.708	0.000e+00	0.00658	1.117	1.743
hon_000_06562	Sn ₄ Tb ₂	6	-4.284	-4.579	-1.000e-06	0.00838	1.406	1.944
hon_000_06565	AlFe ₂ Ni ₂ Ti	6	-6.423	-6.733	-3.000e-06	0.00475	0.558	1.009
hon_000_06592	Cl ₃ Ge ₂ SYb ₂	8	-3.112	-3.966	-1.100e-05	0.0076	1.858	3.212
hon_000_06601	Er ₂ PbPdRu ₂	6	-5.819	-6.329	1.000e-06	0.00752	0.628	2.14
hon_000_06613	Ga ₂ Ni ₂ PtZn	6	-4.228	-4.312	-3.000e-06	0.00541	0.166	0.23
hon_000_06626	PbSn ₃ Yb ₂	6	-3.426	-3.358	3.000e-06	0.00303	0.849	1.962
hon_000_06628	Ca ₄ Nd ₂	6	-2.756	-2.764	-1.000e-06	0.00234	0.108	0.168
hon_000_06640	Nd ₂ Sn ₄	6	-4.319	-4.546	-1.000e-06	0.00622	0.631	0.381
hon_000_06644	PdSe ₄ Yb ₂	7	-3.622	-4.293	-9.000e-06	0.00448	1.846	1.563

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_06647	CaGd ₂ SnSr	5	-3.12	-3.439	-1.000e-06	0.00581	1.807	3.019
hon_000_06654	Ga ₃ Mn ₃	6	-5.741	-5.848	-1.600e-05	0.00349	0.158	1.828
hon_000_06682	LiNi ₂ S ₂ Zn	6	-3.8	-4.109	-3.000e-06	0.00702	1.152	1.542
hon_000_06685	Fe ₂ PdZn ₄	7	-3.424	-3.67	-1.900e-05	0.00662	0.695	1.062
hon_000_06697	BrCl ₃ Nd ₂	6	-3.202	-4.599	-1.000e-06	0.00433	1.18	2.768
hon_000_06700	K ₃ NaYb ₂	6	-0.992	-1.082	2.300e-06	0.00337	0.802	0.436
hon_000_06742	Al ₄ Fe ₂ Si	7	-4.951	-5.141	4.000e-06	0.00419	0.542	1.049
hon_000_06746	Li ₃ Ni ₂	5	-3.131	-3.227	0.000e+00	0.00408	0.389	1.672
hon_000_06751	Cl ₄ Gd ₂ Ir ₂	8	-4.507	-5.175	-4.600e-05	0.0062	1.507	2.642
hon_000_06773	AuLi ₂ Ru ₂ Sb	6	-4.466	-4.906	1.000e-06	0.00626	0.882	2.241
hon_000_06778	Co ₂ CrMoNiSb	6	-6.95	-7.208	-1.000e-06	0.00436	0.383	0.938
hon_000_06787	Gd ₂ NaP ₂ S ₃	8	-4.16	-5.259	-7.000e-06	0.0094	1.676	2.752
hon_000_06788	Cd ₃ MgYb ₂	6	-1.013	-1.34	-1.000e-07	0.00314	1.731	1.124
hon_000_06824	Ga ₄ Tb ₂	6	-3.362	-3.742	0.000e+00	0.00756	0.679	1.338
hon_000_06828	Hg ₄ Nd ₂	6	-1.692	-2.019	0.000e+00	0.00233	0.617	1.597
hon_000_06829	AgCd ₂ ErYb ₂	6	-1.679	-2.187	1.000e-06	0.00582	1.033	2.39
hon_000_06863	AlMn ₂ V ₃	6	-7.992	-8.263	-1.000e-06	0.00404	0.605	1.169
hon_000_06887	BiEu ₂ Ru ₂	5	-4.51	-5.449	1.000e-06	0.00548	1.241	1.843
hon_000_06889	HgNaPmRu ₂	5	-4.214	-4.721	0.000e+00	0.0036	0.978	1.697
hon_000_06896	Ga ₂ Gd ₂ Mg ₂	6	-2.925	-3.18	1.000e-06	0.00748	0.475	0.235
hon_000_06910	Al ₂ Fe ₂ Ga ₂ Li ₂	8	-4.015	-4.168	1.000e-06	0.00579	0.321	1.347
hon_000_06922	Ag ₂ Ga ₃ Tb ₂	7	-3.333	-3.687	-2.000e-06	0.00475	1.169	2.972
hon_000_06972	LaNi ₄ Sn ₂	7	-5.021	-5.124	-2.000e-06	0.00684	0.183	1.507
hon_000_06974	Cs ₃ Nd ₂ Pb	6	-2.082	-2.366	-1.000e-06	0.00321	1.56	2.481
hon_000_06998	Sn ₄ Tb ₂	6	-4.322	-4.579	-1.000e-06	0.00685	1.324	1.815
hon_000_07020	Au ₂ Fe ₂ Lu	5	-5.1	-5.474	1.000e-06	0.00563	0.668	2.281
hon_000_07024	Co ₃ Dy ₃ Ga	7	-5.224	-5.617	-5.500e-05	0.00663	1.313	2.712
hon_000_07032	InNa ₃ Yb ₂	6	-1.526	-1.62	-4.000e-07	0.00493	0.881	0.551
hon_000_07075	SbSr ₂ Tb ₂	5	-3.034	-3.559	-7.000e-06	0.00566	1.621	2.923
hon_000_07082	Fe ₃ Pt ₃	6	-6.793	-7.016	0.000e+00	0.00591	0.262	0.355
hon_000_07089	Nd ₂ Sn ₂ YbZn	6	-3.293	-3.838	0.000e+00	0.00481	2.094	1.184
hon_000_07093	Cl ₆ Gd ₂	8	-4.78	-4.819	0.000e+00	0.0057	0.325	1.147
hon_000_07106	Al ₄ Co ₂ Si	7	-4.707	-4.869	-8.000e-06	0.0051	0.534	0.372
hon_000_07132	PtRu ₂ SiZr ₂	6	-7.758	-8.507	3.000e-06	0.00619	0.844	2.458
hon_000_07174	AlEu ₃ Nd ₂	6	-2.976	-3.121	0.000e+00	0.00233	1.149	1.979
hon_000_07180	AlFe ₂ Na ₂ Tl	6	-3.464	-3.879	-4.000e-06	0.00888	1.164	2.075
hon_000_07190	Cl ₄ Pt ₂ Tb ₂	8	-3.844	-5.016	0.000e+00	0.00662	1.123	2.595
hon_000_07211	Sn ₃ Yb ₃	6	-2.918	-3.157	-2.000e-06	0.00517	0.842	0.558
hon_000_07233	AuRu ₃ Tb ₂	6	-6.627	-6.775	-2.000e-06	0.00285	0.459	0.531
hon_000_07234	Ga ₃ Ni ₂ Pd	6	-4.335	-4.459	0.000e+00	0.00509	0.54	0.996
hon_000_07239	Dy ₂ Ho ₂ InLa	6	-4.347	-4.401	0.000e+00	0.0075	0.241	0.219
hon_000_07293	Dy ₂ LaSn ₃	6	-4.529	-4.844	-1.000e-06	0.00644	1.544	1.912
hon_000_07295	Fe ₄ Os ₂	6	-8.996	-9.066	1.000e-06	0.00715	0.138	0.172
hon_000_07303	Gd ₂ NaRu ₂ SnZn	7	-4.492	-5.002	-2.000e-06	0.00459	1.13	1.899
hon_000_07307	Cl ₄ Nd ₂ W	7	-4.521	-5.203	0.000e+00	0.00579	0.72	2.892
hon_000_07332	Al ₂ LiNi ₂ SiZn	7	-3.9	-4.048	-5.000e-06	0.00838	0.38	1.668
hon_000_07353	PrSnSrTb ₃	6	-3.88	-4.079	-1.200e-05	0.00379	0.971	0.709
hon_000_07364	Ag ₃ Tb ₄	7	-3.752	-3.902	5.000e-06	0.00351	0.408	1.287
hon_000_07365	Cl ₄ Gd ₂ Pt ₂	8	-4.091	-4.841	-1.400e-05	0.00353	2.094	2.776
hon_000_07372	Er ₂ In ₂ Ru ₂	6	-5.283	-5.591	-3.000e-06	0.00737	0.526	1.313
hon_000_07428	Fe ₄ SiU	6	-7.795	-8.367	2.000e-06	0.0037	1.24	1.756
hon_000_07450	CaCdNi ₂ Zn	5	-2.663	-2.971	-1.000e-06	0.00529	0.624	0.726

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_07483	Au ₄ Co ₂	6	-3.904	-4.193	8.000e-06	0.00582	1.182	0.868
hon_000_07501	Cl ₄ Dy ₂ Os	7	-4.111	-5.255	-1.000e-06	0.00651	1.706	1.684
hon_000_07529	Rh ₂ Se ₄ Tb ₂	8	-5.093	-5.7	-1.000e-06	0.00445	1.279	1.238
hon_000_07530	C ₂ AlMn ₄	7	-7.741	-8.057	-5.000e-06	0.00724	0.708	1.402
hon_000_07537	BiFeLiNi ₃	6	-4.709	-4.901	6.000e-06	0.00477	0.256	1.15
hon_000_07546	Fe ₂ GaIrLiMg ₂	7	-4.372	-4.601	-2.000e-06	0.00504	0.567	1.831
hon_000_07550	Gd ₂ RbS ₄ Sb	8	-4.434	-5.147	0.000e+00	0.00388	2.306	1.421
hon_000_07564	Dy ₆	6	-4.509	-4.516	0.000e+00	0.00231	0.074	0.066
hon_000_07567	CdGd ₂ MgSc ₂	6	-3.805	-3.968	-9.000e-06	0.00296	0.509	0.514
hon_000_07596	Gd ₄ MgSn	6	-3.859	-4.136	-3.000e-06	0.00713	0.541	0.44
hon_000_07696	Bi ₃ Yb ₃	6	-3.111	-3.426	-1.750e-04	0.00819	1.223	2.844
hon_000_07711	Ca ₂ Nd ₂ Sn	5	-3.203	-3.653	-1.000e-06	0.00517	2.02	2.538
hon_000_07724	NaSr ₂ Yb ₃	6	-1.405	-1.442	-5.400e-06	0.00237	0.268	0.148
hon_000_07768	Nd ₂ RhSe ₄	7	-4.597	-5.708	-2.000e-06	0.00446	1.341	4.018
hon_000_07780	Tb ₂ Tl ₄	6	-3.041	-3.176	-1.000e-06	0.00314	0.474	0.49
hon_000_07783	Al ₂ Fe ₃	5	-5.994	-6.136	1.000e-06	0.00561	0.385	0.31
hon_000_07791	Dy ₂ Sn ₃	5	-4.335	-4.502	1.000e-06	0.00756	0.777	1.639
hon_000_07805	Cl ₆ Nd ₂	8	-4.784	-4.823	0.000e+00	0.00386	0.229	0.23
hon_000_07854	GeNNi ₃	5	-5.58	-5.806	0.000e+00	0.00562	1.083	0.809
hon_000_07856	Ga ₂ NaNi ₂	5	-3.56	-3.659	-7.000e-06	0.00621	0.326	1.15
hon_000_07860	Ga ₂ Mn ₂ Ni ₂	6	-5.502	-5.74	-2.000e-05	0.00749	0.89	1.997
hon_000_07887	CeRu ₂ Si ₂	5	-7.209	-7.51	-2.000e-06	0.00698	0.804	0.521
hon_000_07914	Cs ₃ SbYb ₂	6	-1.564	-1.779	-5.800e-05	0.00835	1.778	1.614
hon_000_07928	Ho ₂ InRu ₂	5	-5.378	-6.074	-1.000e-06	0.00978	0.616	0.555
hon_000_07946	Fe ₂ Na ₃ PtSb	7	-3.757	-4.083	-6.000e-06	0.0073	0.861	0.799
hon_000_08022	Ru ₂ Zr ₄	6	-8.597	-8.9	-1.000e-05	0.00711	0.734	0.582
hon_000_08043	Dy ₄ Li ₂	6	-3.404	-3.573	0.000e+00	0.00671	0.996	0.739
hon_000_08082	AsBr ₄ ClTb ₂	8	-3.99	-4.246	-1.000e-06	0.007	0.706	2.287
hon_000_08083	Fe ₂ OscSi ₂	6	-7.294	-7.633	2.000e-06	0.00878	1.278	2.625
hon_000_08084	Br ₃ GeITb ₂	7	-2.479	-4.077	-1.000e-06	0.00566	1.398	3.086
hon_000_08092	Cl ₄ PdTb ₂	7	-3.907	-4.601	-2.000e-06	0.00506	1.694	2.426
hon_000_08096	H ₂ AlRu ₂ UZn	7	-4.858	-5.95	-1.000e-05	0.00794	1.543	1.104
hon_000_08101	Fe ₄ GaZn	6	-5.755	-5.944	0.000e+00	0.00486	0.467	1.363
hon_000_08128	Co ₂ CuGaLa	5	-4.798	-5.202	-2.000e-06	0.00638	0.701	1.822
hon_000_08163	AuCe ₂ Fe ₂ Ga	6	-5.768	-5.99	-6.000e-06	0.00621	0.585	1.927
hon_000_08207	Co ₂ CuEuGe	5	-4.454	-4.843	0.000e+00	0.00831	0.704	1.775
hon_000_08209	CeCuGaLiNi ₂	6	-4.258	-4.472	-2.400e-05	0.007	0.533	0.434
hon_000_08214	Cl ₄ PdTb ₂	7	-3.585	-4.557	1.000e-06	0.00663	1.591	3.671
hon_000_08230	Co ₄ Ge ₃ Sn	8	-5.182	-5.656	-8.000e-06	0.00867	1.244	1.198
hon_000_08259	Li ₄ Ni ₂ Tb	7	-3.025	-3.149	8.000e-06	0.00448	0.919	1.981
hon_000_08310	Hg ₃ PbYb ₃	7	-1.525	-1.692	0.000e+00	0.00311	1.403	3.173
hon_000_08368	AuRu ₂ SnTi	5	-6.444	-6.683	-1.800e-05	0.0041	0.375	2.096
hon_000_08382	Sn ₂ Yb ₄	6	-2.433	-2.748	-1.100e-05	0.0079	1.251	0.682
hon_000_08405	Ni ₃ SiU ₂	6	0.564	-7.653	-2.000e-06	0.00298	0.304	1.711
hon_000_08425	Al ₂ HoNi ₄	7	-5.018	-5.185	-1.400e-05	0.00666	0.204	1.474
hon_000_08441	Gd ₂ LaMg ₂	5	-3.038	-3.232	2.000e-06	0.00326	0.682	0.688
hon_000_08474	BrCl ₃ Gd ₂ Pt	7	-3.636	-4.934	-1.000e-06	0.00441	1.765	2.801
hon_000_08572	Co ₂ NiSi ₃	6	-6.09	-6.264	-1.000e-06	0.00346	0.765	0.652
hon_000_08594	Cd ₂ Gd ₂ MgSr	6	-2.145	-2.458	3.000e-06	0.0029	2.069	2.349
hon_000_08611	DyGd ₂ LaMgSn	6	-4.068	-4.264	0.000e+00	0.00743	0.931	1.772
hon_000_08617	Dy ₂ PS ₃ Se ₂	8	-4.366	-5.34	-3.000e-06	0.00602	1.987	2.3
hon_000_08639	EuMgPb ₂ Yb ₂	6	-2.371	-2.62	-1.000e-06	0.00303	1.023	1.069

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_08641	As ₂ Ru ₂ Th	5	-6.145	-7.497	-1.900e-05	0.00635	0.67	0.791
hon_000_08658	Dy ₂ Sn ₄	6	-4.262	-4.563	0.000e+00	0.00759	1.459	2.055
hon_000_08663	Co ₃ Zr ₅	8	-7.595	-8.109	-2.000e-06	0.00913	1.232	1.775
hon_000_08666	AgDy ₄ Yb	6	-3.599	-3.725	0.000e+00	0.0023	0.807	1.583
hon_000_08672	BaGd ₂ Sr ₂	5	-2.311	-2.629	2.000e-06	0.00335	1.288	3.684
hon_000_08681	Co ₂ Si ₄	6	-5.767	-6.065	-1.000e-06	0.0079	0.593	1.726
hon_000_08707	Ga ₃ Mg ₂ Ni ₃	8	-3.615	-3.763	-1.000e-06	0.00658	0.509	1.653
hon_000_08708	AgCa ₃ MgRu ₂	7	-3.65	-3.941	0.000e+00	0.00587	0.622	1.777
hon_000_08736	Fe ₂ Ga ₂ MgTb ₃	8	-4.484	-4.833	-1.100e-05	0.00423	0.994	2.729
hon_000_08747	Sn ₃ Tb ₃	6	-4.489	-4.842	-1.900e-05	0.00887	0.8	1.884
hon_000_08753	AlDy ₂ Fe ₂ Li	6	-5.039	-5.172	-1.000e-06	0.00697	1.133	1.293
hon_000_08785	Co ₃ LiMnSn ₃	8	-4.93	-5.255	-1.000e-06	0.00545	0.73	1.0
hon_000_08808	BrCl ₃ Dy ₂ Pt ₂	8	-3.902	-4.71	1.000e-06	0.00698	2.301	4.13
hon_000_08817	Al ₂ Ge ₂ Nd ₂ PrTh	8	-4.744	-5.312	-3.100e-05	0.0058	1.647	1.879
hon_000_08830	CoGd ₆	7	-4.906	-4.956	0.000e+00	0.00387	0.183	0.183
hon_000_08839	IrNbNd ₂ Se ₄	8	-5.636	-6.293	-4.000e-06	0.00545	1.461	1.052
hon_000_08848	Al ₃ Co ₂ CuDy	7	-4.699	-4.963	-7.000e-06	0.00752	0.341	0.998
hon_000_08894	Cs ₄ Yb ₂	6	-0.721	-0.838	0.000e+00	0.0016	0.825	0.703
hon_000_08898	AlCdDy ₂ Th ₂	6	-4.595	-4.849	-2.000e-06	0.00374	0.725	1.13
hon_000_08905	Cs ₄ Yb ₂	6	-0.762	-0.86	-2.787e-04	0.00816	1.137	2.013
hon_000_08916	GaPtPu ₂ Ru ₂	6	-8.788	-9.285	0.000e+00	0.00351	1.11	1.369
hon_000_08934	Ni ₄ PtU	6	-6.733	-6.862	-2.000e-06	0.00512	0.261	0.314
hon_000_08938	Au ₂ Na ₂ Ru ₂ Sb	7	-3.993	-4.333	-6.000e-06	0.00429	0.831	1.506
hon_000_08964	Eu ₂ In ₂ Ru ₂	6	-4.276	-4.684	-2.000e-06	0.00867	0.645	2.428
hon_000_08973	HGeRu ₂ ScU	6	-7.047	-7.623	-3.000e-06	0.00693	1.389	0.951
hon_000_08996	Co ₂ Ga ₂ Pt ₂	6	-5.106	-5.531	0.000e+00	0.00784	0.425	1.005
hon_000_09007	NaSbSn ₃ Tb ₂	7	-3.759	-4.048	-2.000e-06	0.00466	1.169	2.531
hon_000_09013	CdGd ₃ InTb	6	-3.745	-3.758	-9.000e-06	0.00523	0.284	0.306
hon_000_09020	Ge ₂ MgMn ₄	7	-6.022	-6.457	1.000e-06	0.00468	0.92	1.353
hon_000_09024	Cl ₆ Gd ₂	8	-4.753	-4.82	0.000e+00	0.00496	0.319	0.373
hon_000_09037	Dy ₃ ScSn ₂	6	-4.611	-5.035	-2.000e-06	0.00705	1.288	1.835
hon_000_09043	AuLa ₂ PbRu ₂	6	-5.855	-6.061	-4.000e-06	0.00383	0.656	1.38
hon_000_09045	AuClGd ₂ I ₃	7	-2.856	-3.895	-6.000e-06	0.00582	1.984	3.978
hon_000_09048	Gd ₄ Mg ₂	6	-3.472	-3.612	-3.000e-06	0.00195	0.981	2.632
hon_000_09059	H ₃ Mn ₂ Sc	6	-4.674	-5.793	-1.000e-06	0.00808	0.885	2.219
hon_000_09077	GaNi ₄ Si	6	-5.356	-5.382	-2.000e-06	0.00783	0.057	1.506
hon_000_09105	AsCo ₂ GeNdPt	6	-5.059	-5.998	-1.000e-06	0.00766	0.989	2.756
hon_000_09107	Co ₃ GaU ₂	6	-9.354	-7.845	-1.500e-05	0.00803	0.124	0.839
hon_000_09114	CdCs ₃ Yb ₂	6	-0.842	-0.878	-8.000e-07	0.00294	0.301	2.702
hon_000_09168	Cl ₄ Dy ₂ Ti ₂	8	-4.379	-5.003	-2.000e-06	0.0034	1.296	4.575
hon_000_09170	Al ₄ Ru ₂	6	-5.387	-5.99	3.000e-06	0.00606	0.89	2.013
hon_000_09183	Eu ₂ InYb ₃	6	-1.812	-1.938	-2.000e-06	0.00389	1.332	2.901
hon_000_09206	Co ₂ GdGePt	5	-5.628	-6.201	-7.600e-05	0.00868	0.46	1.505
hon_000_09208	CePb ₃ Tb ₂	6	-4.424	-4.524	-1.000e-06	0.0035	0.543	1.549
hon_000_09237	K ₄ Nd ₂	6	-1.664	-1.803	4.000e-06	0.00294	1.03	2.076
hon_000_09251	Ni ₃ P ₂ Si	6	-5.201	-5.686	-1.300e-05	0.00432	1.107	0.814
hon_000_09269	AlFe ₂ Mg ₂ Pd	6	-4.434	-4.739	-1.000e-06	0.00405	0.758	2.029
hon_000_09271	Ga ₃ NpRu ₂	6	-6.289	-6.695	2.000e-06	0.0055	0.647	0.557
hon_000_09287	Bi ₂ EuIrNd ₂ Si	7	-4.975	-5.372	0.000e+00	0.00486	0.61	0.722
hon_000_09290	AsNi ₃ PtSr ₂	7	-4.606	-4.861	-5.500e-05	0.00987	0.42	1.98
hon_000_09294	Cl ₄ Cr ₂ Gd ₂	8	-4.496	-5.356	0.000e+00	0.00871	2.15	3.342
hon_000_09303	Ca ₂ CdGd ₂ Ge ₃	8	-3.245	-3.995	-1.000e-06	0.00554	1.477	1.521

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_09312	Fe ₃ GeSi ₂	6	-6.617	-6.85	-4.500e-05	0.00959	0.33	1.12
hon_000_09321	Cs ₄ Yb ₂	6	-0.704	-0.837	-2.400e-06	0.00188	0.913	0.957
hon_000_09360	Al ₂ Co ₂ LiY	6	-4.845	-5.067	-2.200e-05	0.00719	0.887	0.922
hon_000_09364	GaNi ₄ Sn	6	-4.856	-4.961	-6.000e-06	0.00506	0.34	0.299
hon_000_09391	CuEr ₂ Fe ₂ Ga	6	-5.353	-5.508	-5.000e-06	0.00851	0.394	0.406
hon_000_09398	AlNi ₃ Rh ₂	6	-5.798	-5.976	0.000e+00	0.00624	0.304	0.917
hon_000_09418	Hf ₄ Nd ₂	6	-7.623	-7.929	3.000e-06	0.00499	0.51	0.244
hon_000_09439	Co ₃ Ga ₃	6	-4.976	-5.02	0.000e+00	0.00318	0.166	0.103
hon_000_09450	Ce ₃ Ni ₄	7	-5.876	-5.916	1.000e-06	0.00571	0.576	0.589
hon_000_09451	Co ₃ Dy ₂ MgSi	7	-5.284	-5.364	-4.200e-05	0.008	0.241	1.439
hon_000_09468	K ₂ RbYb ₂	5	-0.813	-1.004	-1.040e-05	0.00563	1.79	2.592
hon_000_09483	Sn ₃ YYb ₂	6	-3.531	-4.15	-1.700e-05	0.00718	1.371	2.741
hon_000_09535	Sn ₄ Tb ₂	6	-4.212	-4.619	3.000e-06	0.0038	1.909	1.767
hon_000_09557	AuBa ₂ PdSn ₂ Yb ₂	8	-3.339	-3.419	-2.000e-06	0.00348	0.359	0.438
hon_000_09587	NaRb ₂ Yb ₂	5	-0.777	-1.034	3.000e-07	0.00197	1.055	2.331
hon_000_09588	Cd ₂ Co ₂ Li ₂	6	-2.869	-3.033	-6.000e-06	0.00885	0.656	3.178
hon_000_09593	Ga ₃ Ru ₂ Zr	6	-6.019	-6.21	-3.000e-06	0.00792	1.029	0.638
hon_000_09594	Cl ₄ Ir ₂ Nd ₂	8	-4.516	-5.208	-1.000e-06	0.0054	1.698	1.065
hon_000_09651	Ga ₅ Nd ₃	8	-3.863	-4.156	-2.000e-06	0.00927	0.651	0.482
hon_000_09689	CaSbTb ₂ Tl	5	-3.453	-4.0	-1.000e-06	0.00358	2.095	1.184
hon_000_09691	Cl ₄ WYb ₂	7	-3.74	-4.35	-5.000e-06	0.00395	1.665	0.97
hon_000_09730	Ga ₄ Ni ₂	6	-3.585	-4.027	-1.000e-06	0.00634	1.047	1.76
hon_000_09735	Cl ₄ IrTb ₂	7	-3.974	-4.955	2.000e-06	0.00573	1.434	1.462
hon_000_09736	Al ₃ Ru ₂ Tb ₂	7	-5.432	-5.716	0.000e+00	0.00559	0.67	1.259
hon_000_09737	Gd ₄ LiSn	6	-4.016	-4.157	6.000e-06	0.00437	0.649	2.296
hon_000_09740	I ₂ Tb ₂	4	-2.919	-3.704	-7.000e-06	0.0038	1.533	2.637
hon_000_09742	GaGd ₂ SnUZr	6	-5.687	-5.952	-2.000e-06	0.0047	0.71	2.512
hon_000_09744	GaLi ₂ PdRu ₂	6	-5.125	-5.197	-1.000e-06	0.00683	0.233	1.127
hon_000_09847	CuGaNi ₂ Tb ₂	6	-4.823	-4.874	-2.000e-06	0.004	0.32	0.953
hon_000_09857	Dy ₃ PdRu ₂	6	-6.117	-6.481	-7.000e-06	0.00403	1.252	2.36
hon_000_09917	Ni ₄ Sn ₂	6	-4.722	-4.869	-2.000e-05	0.00746	0.198	0.392
hon_000_09928	Dy ₂ Gd ₂ Sn ₂	6	-4.49	-4.771	-2.000e-06	0.0057	1.779	1.515
hon_000_09929	AlCr ₂ GaMn ₂	6	-6.934	-7.232	-5.000e-05	0.00944	0.44	1.991
hon_000_09936	Ce ₃ PtRu ₂	6	-7.135	-7.383	-2.000e-06	0.0084	0.275	1.163
hon_000_09941	Fe ₂ Gd ₂ PdTl	6	-5.449	-5.703	-5.000e-06	0.0096	1.282	2.015
hon_000_09942	KNd ₂ RhSn ₃	7	-4.139	-4.566	1.000e-06	0.00812	1.114	1.727
hon_000_09947	AlNi ₂ Os ₂ W	6	-8.343	-8.391	-1.300e-05	0.00628	0.094	0.15
hon_000_09962	CaSnTb ₄	6	-4.023	-4.156	0.000e+00	0.00395	0.495	0.235
hon_000_09965	Ca ₂ MgTb ₃	6	-3.014	-3.083	-1.000e-06	0.00148	0.403	2.448
hon_000_10007	Dy ₂ MgSn ₃	6	-3.936	-4.153	-2.600e-05	0.00794	1.02	2.432
hon_000_10030	HgNd ₂ PdRu ₂	6	-5.511	-5.81	-3.000e-06	0.00497	0.578	2.113
hon_000_10031	Al ₃ GaMgNi ₂	7	-3.821	-4.024	-1.000e-06	0.00671	0.33	2.155
hon_000_10067	Ga ₃ Ni ₂ Pd	6	-4.387	-4.46	-5.000e-06	0.00797	0.246	0.137
hon_000_10079	Al ₂ GeRu ₂ U	6	-6.813	-7.016	-2.000e-06	0.00879	0.42	0.471
hon_000_10140	Br ₄ Ir ₂ Nd ₂	8	-4.344	-4.929	0.000e+00	0.00312	1.571	1.325
hon_000_10143	PbSn ₃ Yb ₂	6	-3.51	-3.4	8.000e-06	0.00445	1.098	1.573
hon_000_10189	Eu ₃ Ru ₂ Sn	6	-4.237	-4.784	-2.000e-06	0.00455	0.833	1.469
hon_000_10267	CuGd ₂ Ru ₂ Sb	6	-5.852	-6.293	5.000e-06	0.0053	0.687	1.335
hon_000_10269	AsFe ₃ NbPt ₂ Si	8	-6.885	-7.313	0.000e+00	0.00379	0.534	1.639
hon_000_10295	H ₄ Mn ₂ Zr	7	-4.772	-5.804	-3.000e-06	0.00321	0.839	1.102
hon_000_10303	Pd ₂ S ₃ SeTb ₂	8	-4.693	-5.674	0.000e+00	0.00274	2.303	3.194
hon_000_10312	AgDy ₂ GeTl ₄	8	-3.259	-3.335	-4.000e-06	0.00355	0.757	0.437

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_10331	CdMgNd ₃ Pd ₂ Sn	8	-4.075	-4.273	-4.000e-06	0.00616	0.891	2.17
hon_000_10335	Fe ₂ GaLaSnTm	6	-4.889	-5.499	0.000e+00	0.00713	1.194	1.359
hon_000_10341	CaSn ₃ Yb ₂	6	-2.912	-3.264	2.000e-06	0.00585	1.157	1.897
hon_000_10363	Co ₃ FeMo ₂	6	-8.227	-8.441	2.000e-06	0.00382	0.222	0.906
hon_000_10374	Al ₂ Ni ₂ Sc ₃	7	-5.359	-5.777	-1.700e-05	0.00515	0.888	2.585
hon_000_10377	Ce ₂ GaPbRu ₂	6	-6.042	-6.331	-2.000e-06	0.00717	0.816	1.563
hon_000_10404	HCaMn ₂ Os	5	-5.578	-6.563	-5.600e-05	0.00916	0.939	2.59
hon_000_10406	Co ₂ SmSn ₃	6	-4.659	-5.183	0.000e+00	0.0074	0.847	1.482
hon_000_10414	GeLiMn ₂ SiTb	6	-5.349	-5.897	0.000e+00	0.00648	0.709	1.973
hon_000_10429	Co ₃ NiTb	5	-5.755	-6.122	-1.000e-06	0.00774	0.695	0.699
hon_000_10478	Dy ₂ Gd ₃ Mg	6	-3.946	-4.027	-9.000e-06	0.00502	0.453	0.434
hon_000_10489	Ge ₂ LiRu ₂ Zr	6	-6.285	-6.575	-1.000e-06	0.00833	1.076	2.029
hon_000_10549	AlCo ₂ FeLiPt	6	-5.563	-5.779	-6.000e-06	0.00489	1.085	1.707
hon_000_10555	AlMn ₂ Y ₂	5	-5.793	-6.583	-2.000e-06	0.00714	0.76	0.776
hon_000_10556	BaDy ₂ PbTl	5	-3.127	-3.566	-5.000e-06	0.00552	0.833	2.239
hon_000_10579	La ₂ NaTb ₃	6	-3.912	-3.97	2.000e-06	0.00811	0.509	0.46
hon_000_10654	GeMn ₂ Pd ₂ Zn	6	-5.425	-5.623	-1.000e-06	0.00599	1.024	1.405
hon_000_10658	Fe ₂ Pd ₂ Sn	5	-5.73	-5.987	1.000e-06	0.00861	0.613	0.47
hon_000_10678	Ga ₃ Ni ₂ Pd	6	-4.236	-4.435	-2.000e-06	0.00706	0.326	0.925
hon_000_10691	AlPdRu ₂ Tb ₂	6	-6.217	-6.494	-1.000e-06	0.00384	0.45	1.173
hon_000_10694	AlGaMn ₂ Pd	5	-5.61	-6.033	-1.000e-06	0.0074	1.145	1.519
hon_000_10702	Cl ₄ Gd ₂ Mo	7	-4.271	-5.005	-5.000e-06	0.0026	1.587	4.281
hon_000_10707	PrSn ₂ Tb ₃	6	-4.545	-4.692	-2.000e-06	0.00201	0.321	1.41
hon_000_10721	Nd ₂ Se ₄ Si ₂	8	-4.445	-5.209	-1.000e-06	0.00508	1.693	3.643
hon_000_10728	DyNa ₃ Nd ₂	6	-2.711	-2.763	-4.000e-06	0.00428	0.303	0.287
hon_000_10763	AlNa ₃ Ru ₂ Sb	7	-3.783	-4.121	0.000e+00	0.00662	1.369	1.165
hon_000_10787	HfRu ₂ SnZn	5	-6.19	-6.773	-1.000e-06	0.00628	1.22	2.545
hon_000_10789	HAuMn ₂ Sn	5	-4.218	-5.236	0.000e+00	0.00833	1.054	0.6
hon_000_10801	Ga ₃ Ru ₂ Zr	6	-6.028	-6.228	-6.000e-06	0.00715	1.158	1.469
hon_000_10821	DyHgPrTbYb ₂	6	-2.707	-2.9	-2.000e-06	0.00265	1.351	1.8
hon_000_10825	Ba ₂ Nd ₂ Tl	5	-2.728	-3.078	0.000e+00	0.00521	2.082	3.684
hon_000_10839	Gd ₃ Sn ₂ Zr	6	-4.89	-5.42	-2.000e-06	0.00562	1.752	1.392
hon_000_10872	Cl ₃ CsPtTb ₂	7	-3.488	-4.583	0.000e+00	0.00338	1.999	3.666
hon_000_10881	Fe ₂ SiTm ₂ Zn	6	-5.29	-5.567	3.000e-06	0.00349	0.709	1.423
hon_000_10913	GeLi ₂ Ni ₂	5	-3.636	-3.926	1.000e-06	0.00421	0.415	2.214
hon_000_10914	AuLiMn ₂ NiScSn	7	-5.38	-5.553	-9.000e-06	0.00772	0.55	1.255
hon_000_10931	AlCrFe ₂ Sn ₃	7	-5.268	-5.529	0.000e+00	0.00822	0.469	0.521
hon_000_10938	AgCeRu ₂ Sn	5	-5.789	-6.166	-7.000e-06	0.0091	0.524	0.385
hon_000_10951	Al ₂ Co ₃ Si	6	-5.658	-5.917	-1.500e-05	0.00873	0.497	0.988
hon_000_10952	Pd ₃ Sn ₂ Tb ₃	8	-4.975	-5.305	-1.000e-06	0.00463	0.664	0.574
hon_000_10971	Au ₃ Co ₃ Er	7	-4.153	-4.878	4.000e-06	0.00455	0.731	1.033
hon_000_11004	Ga ₃ Ni ₂ Sc	6	-4.358	-4.757	1.000e-06	0.00613	0.629	0.827
hon_000_11061	KRbSbTb ₂ Tl	6	-2.614	-3.084	-2.000e-06	0.00468	1.166	1.97
hon_000_11107	Al ₄ Dy ₃ Mg	8	-3.738	-4.084	0.000e+00	0.00319	0.862	1.381
hon_000_11116	KNa ₂ PbTb ₂	6	-2.37	-2.65	0.000e+00	0.00473	1.457	0.959
hon_000_11117	Ni ₂ SbSnZr	5	-5.382	-5.821	-1.000e-06	0.00372	0.65	1.441
hon_000_11154	BaCo ₂ Sn ₃ Yb ₂	8	-3.792	-4.062	-2.000e-06	0.00639	0.583	0.968
hon_000_11166	Al ₂ Co ₃ Ge	6	-5.577	-5.744	1.000e-06	0.00456	0.961	1.422
hon_000_11184	Dy ₃ Ga ₂ Sb	6	-4.036	-4.575	-1.000e-06	0.00822	1.328	1.514
hon_000_11225	C ₂ B ₂ Mn ₂ UZr	8	-8.188	-8.807	-2.900e-05	0.00757	0.53	0.393
hon_000_11257	Dy ₅ Mg	6	-3.955	-4.001	-3.000e-06	0.00256	0.167	0.224
hon_000_11271	CdNd ₂ Ru ₂ Sn	6	-5.389	-5.577	0.000e+00	0.00449	0.726	2.28

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E_{start}	E_{final}	E_{conv}	F_{max}	d_{latt}	d_{xy}
hon_000_11278	AuPdRu ₂ Yb ₂	6	-4.914	-5.183	2.000e-06	0.00541	0.441	0.339
hon_000_11312	AuEr ₂ GaRu ₂	6	-5.848	-5.999	-3.000e-06	0.00812	0.418	1.039
hon_000_11334	Fe ₂ Pt ₃ Zr	6	-7.248	-7.507	-3.000e-06	0.00383	0.705	1.227
hon_000_11362	Al ₄ Co ₂ Mn ₂	8	-5.427	-6.006	-1.000e-06	0.00642	1.36	1.556
hon_000_11365	Co ₃ CuNd ₂	6	-5.495	-5.728	-5.000e-06	0.00838	0.647	1.296
hon_000_11410	AgLa ₂ Ru ₂ SbSi	7	-5.522	-5.849	5.000e-06	0.00746	1.034	2.068
hon_000_11440	AlNi ₂ Pt ₂ Si	6	-5.307	-5.935	-1.000e-05	0.00664	0.948	2.248
hon_000_11452	CsGaIn ₂ Sn	6	-3.181	-3.62	-1.000e-05	0.00866	0.571	1.546
hon_000_11463	CaGd ₄ Zr	6	-4.487	-4.653	-5.000e-06	0.00382	0.673	0.458
hon_000_11487	AlDy ₂ GaRu ₂	6	-5.354	-5.981	1.000e-06	0.00561	1.125	1.611
hon_000_11511	Nd ₂ Sn ₃ Tl	6	-3.994	-4.394	0.000e+00	0.00251	1.785	1.639
hon_000_11519	Mn ₂ SiSn ₂	5	-4.515	-5.816	1.000e-06	0.00626	0.863	1.57
hon_000_11529	As ₂ Fe ₂ GaLi ₂	7	-4.618	-4.805	0.000e+00	0.00351	0.297	0.393
hon_000_11549	Al ₃ Ga ₂ Mn ₂ Nb	8	-5.372	-5.622	-5.000e-06	0.00871	0.754	1.428
hon_000_11586	Fe ₂ InTm ₂	5	-5.343	-5.782	1.000e-06	0.00676	1.163	1.242
hon_000_11588	Pd ₂ Ru ₃ W	6	-8.429	-8.493	-1.200e-05	0.00592	0.141	0.859
hon_000_11593	Cd ₂ Ce ₂ Ru ₂	6	-5.266	-5.423	-3.000e-06	0.00534	0.492	1.146
hon_000_11595	SbScSrYb ₃	6	-2.73	-2.975	-2.000e-06	0.00306	1.048	1.829
hon_000_11609	Al ₂ CrCu ₂ Ni ₂ P	8	-4.945	-5.211	-1.100e-05	0.00683	0.303	0.608
hon_000_11622	Dy ₃ Tb ₃	6	-4.473	-4.528	-1.000e-06	0.00132	0.331	0.342
hon_000_11647	Dy ₅ Hg	6	-3.757	-3.868	-1.000e-06	0.00181	0.669	2.386
hon_000_11668	Dy ₂ Te ₄	6	-3.977	-4.701	0.000e+00	0.00407	1.358	1.313
hon_000_11669	Nd ₂ SnSrTl	5	-3.25	-3.683	1.000e-06	0.005	1.556	1.495
hon_000_11717	Br ₄ Dy ₂ Pt	7	-3.321	-4.541	-1.000e-06	0.00526	0.978	4.143
hon_000_11729	AlAuDy ₂ GaSn ₂ Y	8	-4.351	-4.652	-1.000e-06	0.00605	0.942	0.757
hon_000_11732	LaNaSbYb ₃	6	-2.464	-2.776	-1.100e-05	0.0081	1.433	1.24
hon_000_11761	Cd ₂ Gd ₄	6	-3.299	-3.397	-1.000e-06	0.00369	0.295	0.314
hon_000_11764	Mn ₂ OsSn ₄	7	-5.389	-5.988	-1.000e-06	0.00791	0.754	0.97
hon_000_11771	Nd ₂ Sn ₄	6	-4.263	-4.605	-2.000e-06	0.00591	0.601	1.48
hon_000_11785	AgEr ₂ Ru ₂ Sn	6	-5.775	-5.901	-1.000e-06	0.00875	0.302	1.889
hon_000_11818	NdPr ₂ Ru ₂ Sn	6	-5.581	-6.173	-5.000e-06	0.00571	1.152	2.484
hon_000_11823	Au ₂ Co ₂ NiSn	6	-4.481	-4.711	2.000e-06	0.00841	0.525	1.837
hon_000_11855	GePt ₃ Ru ₂	6	-6.68	-6.823	-2.000e-06	0.00894	0.56	1.297
hon_000_11904	AuCo ₃ La ₂	6	-5.759	-5.826	-7.000e-06	0.00764	0.319	0.879
hon_000_11905	Nd ₂ SnTe ₄	7	-3.866	-4.627	1.000e-06	0.00558	1.218	2.419
hon_000_11918	Al ₃ CoDy ₃ Ga	8	-4.457	-4.715	0.000e+00	0.00834	0.971	1.764
hon_000_11923	CaCe ₃ Yb ₂	6	-3.387	-3.528	-3.800e-05	0.00712	0.651	0.365
hon_000_11930	GaTl ₃ Yb ₂	6	-2.164	-2.397	-3.000e-06	0.00414	1.575	1.658
hon_000_11947	Cs ₃ TlYb ₂	6	-1.056	-1.187	-4.900e-06	0.00322	1.529	3.209
hon_000_11949	Ru ₂ TeZr ₂	5	-7.665	-8.056	0.000e+00	0.00649	0.757	1.455
hon_000_11953	Al ₄ PrRu ₂	7	-5.401	-5.608	-1.300e-05	0.00964	0.65	1.235
hon_000_11972	AllIrNd ₂ S ₄	8	-5.276	-6.0	0.000e+00	0.0073	0.834	1.511
hon_000_11976	BaCdGd ₂ K ₂	6	-1.852	-2.076	-1.000e-06	0.0022	1.503	3.299
hon_000_11977	Al ₃ Co ₂	5	-4.91	-5.13	-3.000e-06	0.00565	0.52	1.391
hon_000_11983	Co ₂ Ga ₃	5	-4.46	-4.671	-5.000e-06	0.00526	0.874	0.554
hon_000_12003	Au ₂ Cl ₄ Gd ₂	8	-3.153	-4.336	1.000e-06	0.00458	1.682	3.65
hon_000_12020	La ₃ Tb ₂ Tl	6	-4.277	-4.386	-2.000e-06	0.00707	0.411	1.306
hon_000_12096	Ga ₃ Ni ₂ Pd	6	-4.284	-4.458	-3.000e-06	0.00606	0.52	2.584
hon_000_12105	Al ₂ Fe ₂ SiV	6	-6.208	-6.635	-2.000e-05	0.00796	0.923	2.693
hon_000_12110	DyRu ₃ SnZn	6	-6.043	-6.201	3.000e-06	0.00974	0.307	0.309
hon_000_12118	Gd ₂ Pd ₂ Se ₄	8	-4.558	-5.352	-1.000e-06	0.00419	2.16	2.137
hon_000_12120	Fe ₄ NiSi	6	-7.31	-7.39	-2.000e-06	0.00681	0.164	0.085

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_12149	Fe ₂ Ni ₃ Si	6	-6.402	-6.5	-1.200e-05	0.00829	0.203	0.942
hon_000_12159	Al ₂ Co ₂ La	5	-4.983	-5.432	-3.000e-06	0.0059	0.621	3.132
hon_000_12163	Co ₄ Ni ₂	6	-6.182	-6.328	2.000e-06	0.00483	0.341	0.283
hon_000_12179	Br ₄ Gd ₂ Ti ₂	8	-4.159	-4.696	-7.000e-06	0.00684	1.768	2.401
hon_000_12180	Dy ₄ GaRh ₂	7	-5.228	-5.516	-3.000e-06	0.00735	0.577	1.268
hon_000_12201	Ga ₄ Ru ₂	6	-4.83	-5.147	-1.000e-06	0.00771	0.873	0.833
hon_000_12208	Gd ₂ SbSrTe	5	-3.836	-4.485	-4.000e-06	0.00683	1.7	2.613
hon_000_12210	Au ₂ BiNi ₂	5	-4.04	-4.135	7.000e-06	0.00646	0.372	0.246
hon_000_12219	Mn ₂ V ₃	5	-8.46	-8.8	-1.000e-06	0.00237	0.517	1.204
hon_000_12222	NaNd ₂ Sn ₃	6	-3.77	-4.103	3.000e-06	0.00909	0.978	1.858
hon_000_12247	Tb ₂ Te ₃	5	-3.681	-5.101	0.000e+00	0.00504	2.135	3.537
hon_000_12264	Al ₄ Fe ₂ Sn	7	-4.733	-4.894	-2.000e-06	0.00654	0.603	1.252
hon_000_12278	Ce ₂ Ru ₂ Tl	5	-6.442	-6.695	-2.000e-06	0.0076	0.549	1.326
hon_000_12281	CaDy ₂ Li ₂ Mg	6	-2.502	-2.638	0.000e+00	0.00398	0.639	1.772
hon_000_12289	Nd ₂ Tl ₄	6	-3.056	-3.368	0.000e+00	0.00369	1.411	2.923
hon_000_12292	Cs ₃ Nd ₂ Sn	6	-2.1	-2.446	1.000e-06	0.00521	1.507	3.773
hon_000_12294	Cl ₄ MnTb ₂	7	-3.991	-4.733	0.000e+00	0.00662	1.572	2.044
hon_000_12295	CuFe ₂ GaNd ₂	6	-5.349	-5.498	-1.000e-06	0.00769	0.657	1.294
hon_000_12305	Al ₂ Fe ₂ NiTi	6	-6.178	-6.431	-9.000e-06	0.00464	0.663	1.927
hon_000_12309	Ni ₂ PtTiTm	5	-6.103	-6.32	5.000e-06	0.00797	0.49	1.905
hon_000_12315	EuNa ₂ SbTb ₂	6	-2.729	-3.132	1.000e-06	0.0029	1.57	2.244
hon_000_12332	Ca ₃ Tb ₃	6	-3.058	-3.113	-1.000e-06	0.00094	0.678	0.841
hon_000_12372	Br ₃ PdTb ₂	6	-3.5	-4.476	-4.000e-06	0.00897	2.453	2.73
hon_000_12407	Al ₃ Ni ₂ Zn	6	-3.918	-4.202	1.000e-06	0.00575	0.768	1.34
hon_000_12411	BaCs ₃ Yb ₂	6	-0.867	-1.001	-1.850e-05	0.00136	1.283	3.415
hon_000_12418	Al ₂ Ru ₂ Sn	5	-5.732	-5.904	-1.000e-06	0.00771	0.346	0.237
hon_000_12428	Mn ₂ Pt ₄	6	-6.602	-7.109	-2.000e-06	0.00437	0.657	0.432
hon_000_12462	Cs ₃ Dy ₂	5	-1.471	-1.83	-1.020e-05	0.00847	3.638	4.335
hon_000_12467	AuCrMo ₂ Ru ₂	6	-8.441	-8.613	-5.000e-06	0.0018	0.188	0.232
hon_000_12490	Br ₄ Dy ₂ Pt	7	-3.507	-4.129	-1.000e-06	0.00511	0.855	1.014
hon_000_12494	Cs ₄ Yb ₂	6	-0.743	-0.856	-1.000e-07	0.00165	0.814	3.179
hon_000_12522	Nd ₂ SbSr ₃	6	-3.102	-3.206	1.000e-06	0.00337	0.745	2.637
hon_000_12537	Dy ₆	6	-4.387	-4.511	0.000e+00	0.00059	0.79	0.626
hon_000_12572	GaNd ₂ Sr ₂ Tl	6	-3.014	-3.18	0.000e+00	0.00396	1.12	0.655
hon_000_12579	Co ₃ GeIrRh	6	-6.709	-6.899	1.000e-06	0.00651	0.439	0.385
hon_000_12588	F ₆ Mn ₂	8	-5.057	-5.568	-1.200e-05	0.00788	1.132	1.469
hon_000_12684	Lu ₂ Ru ₂ Sb	5	-5.802	-6.673	-4.000e-06	0.0091	0.911	0.906
hon_000_12689	Ru ₂ Sn ₂ Zr	5	-6.253	-6.894	0.000e+00	0.00484	0.565	0.488
hon_000_12717	Mn ₂ Sb ₂ Sn	5	-5.408	-5.695	-7.000e-06	0.00599	0.453	1.362
hon_000_12763	CaTl ₂ Yb ₂ Zr	6	-2.649	-3.05	0.000e+00	0.00302	1.105	0.798
hon_000_12764	As ₂ GaNi ₂ Sn	6	-4.401	-4.625	-2.000e-06	0.00421	0.662	1.454
hon_000_12770	Br ₆ Tb ₂	8	-4.264	-4.289	0.000e+00	0.00662	0.233	1.104
hon_000_12771	AlFe ₂ HfSiTi ₂	7	-7.189	-7.672	-8.000e-06	0.0048	0.47	0.804
hon_000_12773	CdHfHo ₂ Ru ₂	6	-5.885	-6.289	0.000e+00	0.00527	0.425	1.956
hon_000_12786	CoGeLiNi ₃	6	-4.857	-5.113	-4.000e-06	0.00452	0.485	1.756
hon_000_12792	Lu ₃ Ni ₂ Zn ₂	7	-3.688	-4.13	2.000e-06	0.00641	0.987	1.538
hon_000_12799	Ge ₃ Mn ₂ Pd	6	-5.829	-6.093	-2.900e-05	0.00587	0.396	1.188
hon_000_12816	Ga ₄ Nd ₄	8	-3.906	-4.358	-9.000e-06	0.00766	0.877	0.784
hon_000_12833	Cl ₄ Gd ₂ Ir	7	-3.981	-5.01	1.000e-06	0.00566	1.7	2.173
hon_000_12852	Br ₄ PtYb ₂	7	-2.907	-3.777	-3.000e-06	0.00748	1.323	2.58
hon_000_12901	Br ₅ Gd ₂ Pt	8	-3.462	-4.291	-2.000e-05	0.00982	0.781	2.114
hon_000_12904	FeGe ₃ Ni ₂	6	-5.253	-5.505	0.000e+00	0.006	0.462	1.002

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_12914	Fe ₂ LiMg ₂ Y	6	-4.083	-4.342	0.000e+00	0.00702	1.155	1.389
hon_000_12928	K ₃ Tb ₂ Tl	6	-1.978	-2.172	-8.000e-06	0.00546	2.214	3.804
hon_000_12955	Dy ₂ Ru ₂ Sn	5	-6.259	-6.504	-2.000e-06	0.0061	0.845	0.625
hon_000_12960	GaLiPdRu ₂ Zr	6	-6.179	-6.433	-4.000e-06	0.00588	0.309	1.749
hon_000_12996	Ni ₃ PtSn	5	-5.247	-5.392	1.000e-06	0.00616	0.379	1.097
hon_000_12997	Ce ₃ Ni ₂ RuZn	7	-5.604	-5.775	-1.600e-05	0.0079	0.71	0.938
hon_000_13042	Co ₂ Li ₃ Sn	6	-3.595	-3.898	0.000e+00	0.00771	0.499	0.527
hon_000_13059	Al ₄ CaCo ₂	7	-4.359	-4.45	3.000e-06	0.00889	0.578	1.113
hon_000_13078	Fe ₃ Li ₅	8	-3.431	-3.611	-2.100e-05	0.00575	0.676	1.552
hon_000_13090	Br ₄ RuYb ₂	7	-3.042	-3.85	1.000e-06	0.007	1.663	2.265
hon_000_13094	AsRu ₂ Sc ₂ Zr	6	-7.579	-7.911	-2.000e-06	0.00913	1.074	1.626
hon_000_13095	Co ₃ GeLi ₂ Pt ₂	8	-4.953	-5.225	0.000e+00	0.00415	0.83	2.151
hon_000_13137	Nd ₃ Sn ₅	8	-4.059	-4.636	-1.000e-06	0.00451	1.439	1.248
hon_000_13170	Fe ₂ SiU ₃	6	6.414	-9.225	-8.000e-06	0.00678	0.23	2.661
hon_000_13236	Al ₂ Fe ₂ NiTi	6	-6.209	-6.436	0.000e+00	0.00461	0.449	1.823
hon_000_13281	Al ₂ Ni ₃ Zn	6	-4.428	-4.549	0.000e+00	0.00532	0.478	1.053
hon_000_13283	Co ₄ Ta ₂	6	-8.288	-8.726	-1.600e-05	0.00979	0.924	1.577
hon_000_13300	As ₂ Fe ₂ GaMg ₃	8	-4.018	-4.189	-2.000e-06	0.00375	1.064	2.165
hon_000_13352	Cd ₂ Co ₂ Ge	5	-3.428	-3.763	-1.500e-05	0.00881	0.615	2.005
hon_000_13361	Ca ₂ Dy ₃ Tl	6	-3.118	-3.23	1.200e-05	0.00623	0.356	0.353
hon_000_13364	Ba ₂ RhRuSn ₂ Tb ₂	8	-4.659	-4.922	1.000e-06	0.00237	0.672	1.747
hon_000_13366	Co ₃ La ₂ Si	6	-6.136	-6.334	1.000e-06	0.00494	0.546	1.823
hon_000_13452	BiGd ₂ SbSeTe	6	-4.067	-4.845	0.000e+00	0.00595	1.185	2.015
hon_000_13454	LiNd ₂ Sn ₃	6	-3.999	-4.407	8.300e-05	0.00614	1.154	3.465
hon_000_13516	Na ₃ SbYb ₂	6	-1.894	-2.087	-3.000e-06	0.00517	1.431	2.916
hon_000_13557	AlCd ₂ Co ₂ Li ₂	7	-2.992	-3.144	3.000e-06	0.00914	1.201	2.384
hon_000_13576	Rb ₂ Rh ₂ Se ₂ Yb ₂	8	-3.561	-3.989	-1.000e-06	0.00475	1.636	3.523
hon_000_13646	CaNd ₃ Sn ₂	6	-4.186	-4.393	1.000e-06	0.00292	0.366	1.651
hon_000_13682	Br ₆ Mn ₂	8	-3.485	-3.815	-6.000e-06	0.00656	0.554	0.487
hon_000_13687	Cl ₄ Gd ₂ Ir	7	-4.076	-5.037	-1.000e-06	0.008	1.907	1.503
hon_000_13693	Ga ₄ Mn ₂ Sr	7	-3.725	-4.478	-2.000e-06	0.00571	1.316	2.135
hon_000_13736	Li ₃ PtRu ₂ Sn ₂	8	-4.722	-4.935	-1.000e-06	0.00309	0.345	0.884
hon_000_13739	KMn ₂ S ₃ Yb ₂	8	-4.594	-5.036	0.000e+00	0.00866	0.632	2.344
hon_000_13745	Cs ₄ Yb ₂	6	-0.699	-0.855	-6.400e-06	0.00202	0.957	2.938
hon_000_13780	Al ₂ Fe ₂ Tb	5	-4.526	-5.876	-5.200e-05	0.00872	0.898	0.842
hon_000_13832	CuNi ₄ Ti	6	-5.717	-5.786	2.000e-06	0.00348	0.261	0.302
hon_000_13836	AgGd ₂ Ru ₂ Sn	6	-5.484	-5.913	0.000e+00	0.00324	0.512	1.175
hon_000_13857	Co ₄ GaGe	6	-5.8	-5.923	-2.000e-06	0.00661	0.186	0.84
hon_000_13870	Cd ₂ PbTb ₃	6	-3.019	-3.411	1.000e-06	0.00612	1.342	3.82
hon_000_13888	CaPbTb ₂ Yb ₂	6	-2.933	-3.01	-5.000e-06	0.00401	0.631	1.562
hon_000_13964	AlCa ₂ Dy ₂ Ga	6	-3.163	-3.496	-1.000e-06	0.00122	0.986	2.096
hon_000_13966	ClDy ₂ S ₃ V ₂	8	-5.563	-6.258	0.000e+00	0.00748	0.956	2.483
hon_000_13972	NdSn ₃ Yb ₂	6	-3.232	-3.807	0.000e+00	0.00528	1.189	2.208
hon_000_13997	Sn ₂ Yb ₄	6	-2.407	-2.72	-1.100e-05	0.00626	1.268	3.055
hon_000_14037	Dy ₄ Mg ₂ Pd	7	-3.808	-3.935	1.000e-06	0.00266	0.428	0.646
hon_000_14049	Cl ₆ Nd ₂	8	-4.682	-4.821	-7.000e-06	0.00563	0.466	0.475
hon_000_14054	Ga ₃ IrNi ₂	6	-4.814	-5.016	1.000e-06	0.00672	0.401	1.212
hon_000_14076	NaSn ₃ Yb ₂	6	-2.714	-2.985	-1.000e-05	0.00634	0.634	0.429
hon_000_14094	Cr ₂ Ni ₃ Si	6	-6.798	-6.986	-1.000e-05	0.00574	0.262	0.216
hon_000_14122	CuLi ₄ Ni ₂	7	-3.012	-3.085	4.000e-06	0.00941	0.451	0.45
hon_000_14124	Dy ₂ Ga ₃ MgSnTl	8	-3.13	-3.479	-3.000e-06	0.00897	0.71	1.425
hon_000_14127	Al ₂ Co ₄ Yb	7	-5.019	-5.263	-4.000e-06	0.00759	0.296	0.351

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_14150	CdGaGd ₃ Tl	6	-3.25	-3.555	0.000e+00	0.00675	1.3	3.424
hon_000_14163	Ga ₄ Tb ₂	6	-3.6	-4.032	-9.000e-06	0.00434	0.579	2.402
hon_000_14172	Gd ₂ Ru ₂ SbY	6	-5.733	-6.593	0.000e+00	0.00859	1.283	0.969
hon_000_14180	Nd ₂ Pd ₂ Ru ₃ Sn	8	-6.165	-6.501	-2.000e-06	0.00743	0.749	2.002
hon_000_14222	CoTe ₄ Yb ₂	7	-3.54	-4.018	1.000e-06	0.00281	1.99	2.564
hon_000_14264	Au ₂ Br ₄ Dy ₂	8	-2.875	-4.007	-2.000e-06	0.00968	0.593	2.361
hon_000_14267	Gd ₃ IrSTe ₂	7	-4.979	-5.916	0.000e+00	0.0054	1.278	1.108
hon_000_14271	Cd ₂ Gd ₂ Zr ₂	6	-4.181	-4.535	-1.000e-06	0.00724	0.525	1.495
hon_000_14275	Ca ₄ Gd ₂	6	-2.682	-2.694	2.000e-06	0.00305	0.191	1.194
hon_000_14288	Al ₂ CoFe ₂ Mg	6	-5.275	-5.415	-5.000e-06	0.00472	0.474	1.051
hon_000_14321	Cl ₄ Gd ₂ Ir	7	-4.199	-4.964	-8.000e-06	0.0047	1.719	1.53
hon_000_14326	AlGeNi ₂ Sc ₂	6	-5.465	-5.646	-1.000e-06	0.00462	0.568	1.93
hon_000_14336	Cl ₄ PbTb ₂	7	-3.294	-4.395	-6.000e-06	0.00496	2.242	1.983
hon_000_14338	GaGd ₃ HoMg	6	-3.696	-3.981	-8.000e-06	0.00587	1.21	1.896
hon_000_14346	CdRu ₂ Zn ₂	5	-3.802	-4.024	-6.000e-06	0.00657	0.326	0.162
hon_000_14363	Br ₂ Se ₂ Ti ₂ Yb ₂	8	-3.937	-4.695	-7.000e-06	0.00472	1.7	2.388
hon_000_14366	AsNd ₂ Ru ₂ Zn	6	-5.696	-6.011	-6.000e-06	0.00443	0.795	1.485
hon_000_14369	AuFe ₂ Gd ₂ Sn	6	-5.116	-5.694	-2.100e-05	0.00832	1.593	2.703
hon_000_14406	Co ₄ Si ₂	6	-6.581	-6.801	-3.200e-05	0.00451	0.61	1.107
hon_000_14418	AcCo ₂	3	-5.826	-5.964	-4.500e-05	0.00364	0.279	0.252
hon_000_14434	Al ₃ Fe ₂ Ga	6	-5.024	-5.116	0.000e+00	0.00538	0.216	0.18
hon_000_14438	Cl ₆ Gd ₂	8	-4.649	-4.817	0.000e+00	0.00514	0.695	0.505
hon_000_14451	AsCuNi ₂ Ti ₂	6	-5.975	-6.143	0.000e+00	0.00755	0.558	0.594
hon_000_14457	Ga ₂ Mn ₂ TaZr	6	-6.867	-7.286	1.000e-06	0.00767	0.376	1.004
hon_000_14474	CaCo ₃ Si	5	-5.32	-5.637	-2.000e-06	0.00782	0.392	1.166
hon_000_14475	CaCd ₂ Yb ₃	6	-1.277	-1.494	-2.000e-07	0.0034	1.709	2.394
hon_000_14490	Dy ₃ GdHoIn	6	-4.208	-4.328	0.000e+00	0.00224	0.785	1.431
hon_000_14520	Hf ₂ Rh ₂ Ru ₂	6	-8.702	-9.166	-8.000e-06	0.00552	0.813	1.502
hon_000_14551	AgDy ₃ MgZr	6	-4.147	-4.369	-2.000e-06	0.00388	0.972	1.611
hon_000_14564	Ir ₂ Pb ₂ Tb ₂	6	-5.581	-5.968	-1.000e-06	0.00467	0.585	0.417
hon_000_14602	SbSn ₄ Tb ₂	7	-4.071	-4.515	-6.000e-06	0.0085	1.2	2.161
hon_000_14629	GdNa ₃ Yb ₂	6	-1.688	-1.712	1.000e-06	0.00479	0.252	0.183
hon_000_14631	GaLa ₂ PdRu ₂	6	-6.243	-6.456	-1.200e-05	0.00795	0.585	1.26
hon_000_14638	CoFe ₂ LiNd	5	-5.37	-5.758	-1.000e-06	0.00482	0.41	0.255
hon_000_14660	Gd ₂ La ₃ Sn	6	-4.74	-4.817	0.000e+00	0.00809	0.327	0.36
hon_000_14673	Dy ₂ Te ₂	4	-3.899	-4.968	-9.000e-06	0.00377	1.606	1.24
hon_000_14717	DyNa ₃ Yb ₂	6	-1.636	-1.662	-2.300e-06	0.00505	0.314	1.437
hon_000_14724	Gd ₄ HoMg	6	-3.918	-4.035	0.000e+00	0.00609	0.636	0.52
hon_000_14755	Gd ₂ Ge ₂ Te ₃ Zn	8	-3.771	-4.265	0.000e+00	0.00501	1.107	1.717
hon_000_14806	Dy ₃ Sn ₃	6	-4.431	-4.795	-8.000e-06	0.00656	0.938	0.771
hon_000_14807	AlCo ₂ Ge ₂ Ta	6	-6.151	-6.604	-4.000e-06	0.00843	1.002	2.27
hon_000_14830	Fe ₃ Os ₂ Si	6	-8.434	-8.717	-3.000e-06	0.0061	0.498	1.042
hon_000_14841	Ga ₂ Mn ₂ Pt ₂	6	-5.805	-6.119	-1.000e-06	0.00379	0.281	1.761
hon_000_14847	GaNi ₂ V ₂ Zn	6	-5.539	-5.59	-1.000e-06	0.00377	0.259	0.847
hon_000_14882	Ga ₃ Mn ₂ Ti	6	-5.671	-5.76	0.000e+00	0.00735	0.268	0.913
hon_000_14934	PtRb ₂ Se ₂ Tb ₂	7	-3.418	-4.346	1.000e-06	0.00401	1.946	2.382
hon_000_14945	Ga ₄ Gd ₂ K ₂	8	-2.646	-3.019	0.000e+00	0.00529	1.652	3.169
hon_000_14981	Nd ₂ Sn ₄	6	-4.419	-4.542	1.000e-06	0.00409	0.484	0.479
hon_000_14988	Ru ₂ Se ₄	6	-4.219	-5.439	-2.000e-06	0.00881	0.565	1.209
hon_000_14989	Co ₂ Gd ₂ Sn	5	-5.116	-5.76	0.000e+00	0.00914	1.18	1.176
hon_000_14992	GaRu ₂ Sn ₃	6	-4.901	-5.373	-1.000e-06	0.0037	1.235	0.952
hon_000_15006	Cl ₅ Gd ₂ Na	8	-4.189	-4.268	-2.000e-06	0.00504	0.417	1.999

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_15027	CaCdGd ₂ Mg	5	-2.394	-2.657	-1.000e-06	0.00518	1.719	1.773
hon_000_15034	Co ₄ RhSi	6	-6.843	-6.893	-5.000e-06	0.00845	0.166	0.94
hon_000_15059	AlGaLa ₂ Ru ₂	6	-5.752	-6.088	0.000e+00	0.00535	0.91	1.602
hon_000_15078	LiMgNi ₄	6	-4.171	-4.264	0.000e+00	0.0064	0.478	1.056
hon_000_15110	AsGeNi ₃ W	6	-6.233	-6.424	-1.000e-06	0.00905	0.686	1.453
hon_000_15119	AlGd ₄ SiTl ₂	8	-4.053	-4.367	-9.000e-06	0.00297	0.618	0.508
hon_000_15120	CaGa ₃ Tb ₂	6	-3.291	-3.657	0.000e+00	0.00308	1.083	0.993
hon_000_15128	SSb ₂ Tb ₂ Tl ₂	7	-3.802	-4.45	-1.000e-06	0.00262	2.236	1.826
hon_000_15169	Ge ₂ Na ₃ Ni ₂	7	-2.911	-3.399	-6.000e-06	0.00891	1.298	1.163
hon_000_15183	AlLiRu ₂ SnZr	6	-6.115	-6.313	-2.000e-06	0.00648	0.429	1.835
hon_000_15224	Al ₃ LiRu ₂	6	-5.47	-5.569	-4.000e-06	0.00692	0.286	0.983
hon_000_15232	Co ₂ Pt ₃	5	-5.968	-6.139	-1.000e-06	0.00972	0.178	0.233
hon_000_15236	Cl ₄ Dy ₂ W	7	-4.286	-5.061	-3.000e-06	0.00524	1.092	2.701
hon_000_15249	AgLiMgNd ₂ Sn	6	-3.061	-3.507	0.000e+00	0.00459	1.494	1.778
hon_000_15265	Fe ₄ Ge ₂	6	-6.723	-6.848	-7.600e-05	0.00387	0.548	0.34
hon_000_15273	GeMn ₂ PtU	5	-7.608	-8.254	-1.000e-06	0.00739	0.428	1.45
hon_000_15290	AlFe ₂ GeLu	5	-5.395	-5.776	-1.000e-06	0.00976	0.741	1.489
hon_000_15293	CdRu ₃ VZn	6	-6.035	-6.223	-7.000e-06	0.00828	0.45	1.195
hon_000_15330	LaMg ₃ Nd ₂	6	-3.078	-3.128	-6.000e-06	0.00481	0.336	1.185
hon_000_15343	PrRu ₄ Sn ₃	8	-6.458	-6.584	-4.000e-06	0.00948	0.625	1.177
hon_000_15349	Fe ₂ Ga ₂ PdPt	6	-5.292	-5.654	-3.000e-06	0.00716	0.277	0.228
hon_000_15383	CaCdGd ₂ PdSr ₂	7	-2.927	-3.07	-1.100e-05	0.00894	1.009	0.848
hon_000_15386	FeLi ₂ Ru ₂ Tc	6	-6.398	-6.513	-2.000e-06	0.00241	0.277	0.945
hon_000_15403	Au ₅ Co ₃	8	-4.141	-4.224	1.000e-05	0.00485	0.458	1.261
hon_000_15425	Cl ₃ Nd ₂ Sb	6	-3.352	-4.825	0.000e+00	0.00595	2.639	3.042
hon_000_15441	CuEr ₃ Ru ₂ Zn	7	-5.244	-5.351	3.000e-06	0.00849	0.985	2.438
hon_000_15444	Co ₂ PPtSm	5	-5.942	-6.534	-1.900e-05	0.00737	0.626	1.572
hon_000_15460	Sn ₃ Tb ₃	6	-4.076	-4.847	3.000e-06	0.009	1.714	2.439
hon_000_15475	AgDy ₃ Ga ₄	8	-3.727	-4.009	-2.000e-06	0.00972	0.624	1.553
hon_000_15486	Dy ₂ LiScTb ₂	6	-4.171	-4.259	1.000e-06	0.00422	0.443	1.359
hon_000_15546	Sn ₃ Tb ₂	5	-3.736	-4.411	0.000e+00	0.00818	0.889	3.215
hon_000_15580	Dy ₂ Na ₄	6	-2.011	-2.04	0.000e+00	0.00402	0.406	0.349
hon_000_15592	Ru ₂ SbSm ₂ Sn	6	-5.777	-6.135	0.000e+00	0.00683	0.753	2.069
hon_000_15615	ErMn ₂ NiPd ₂	6	-6.105	-6.481	4.000e-06	0.00995	1.051	2.352
hon_000_15623	GaHf ₃ Ru ₂	6	-8.575	-8.657	-2.100e-05	0.00643	0.336	1.236
hon_000_15624	Be ₂ Ru ₂ Si ₂	6	-6.096	-6.435	-4.000e-06	0.00588	0.846	1.511
hon_000_15630	Co ₂ CuLaSn	5	-4.909	-5.369	0.000e+00	0.00414	0.79	0.983
hon_000_15638	CuRu ₂ YZn ₄	8	-3.983	-4.21	2.000e-06	0.00786	0.335	0.905
hon_000_15640	Al ₅ Tb ₂	7	-3.8	-4.282	0.000e+00	0.00349	1.314	1.695
hon_000_15648	Gd ₂ Mg ₂ Sn ₂	6	-3.414	-3.694	-3.000e-06	0.00322	1.274	1.993
hon_000_15657	Fe ₂ GaHo ₂ Ru ₂	7	-6.402	-6.844	1.000e-06	0.00399	1.015	2.406
hon_000_15677	Fe ₂ Ga ₂ MgSbTb	7	-4.389	-4.587	-4.000e-06	0.00697	1.061	0.984
hon_000_15693	AlCoCuGaNi ₂	6	-4.674	-4.904	-1.000e-06	0.0086	0.997	1.726
hon_000_15748	AuCdFe ₂ LiPt	6	-4.354	-4.566	0.000e+00	0.00396	0.688	1.404
hon_000_15750	BaNd ₂ Te ₃	6	-4.038	-4.957	-1.400e-05	0.00336	2.278	3.131
hon_000_15762	Cl ₆ Nd ₂	8	-4.478	-4.821	-9.000e-06	0.00857	0.901	2.148
hon_000_15769	Cl ₄ PdTb ₂ Y	8	-4.099	-4.896	-4.000e-06	0.00371	0.793	1.216
hon_000_15770	Nd ₂ Pd ₂ S ₄	8	-4.762	-5.882	-3.000e-06	0.00629	1.977	1.956
hon_000_15772	Al ₃ Gd ₃	6	-4.079	-4.351	1.000e-06	0.00642	0.421	1.46
hon_000_15860	Dy ₃ InNa ₂	6	-2.885	-3.058	4.000e-06	0.00198	1.173	2.858
hon_000_15863	Nd ₂ Sn ₄	6	-4.341	-4.545	-3.100e-05	0.00912	0.625	1.31
hon_000_15865	DyFe ₂ Ga ₂ Pd	6	-4.987	-5.599	-1.000e-06	0.00466	0.899	2.67

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_15924	Br ₄ Gd ₂ Pd ₂	8	-3.631	-4.378	-1.000e-06	0.00597	1.361	2.837
hon_000_15933	I ₃ Tb ₂ TlZn	7	-2.404	-3.016	-1.100e-05	0.00486	1.415	1.545
hon_000_15938	DySn ₂ Tb ₃	6	-4.595	-4.663	0.000e+00	0.00338	0.431	0.287
hon_000_15952	Ge ₂ Mn ₂ Zn ₂	6	-4.23	-4.641	1.000e-06	0.00757	0.713	0.446
hon_000_15968	CaMg ₂ Ru ₂ SiZn	7	-4.109	-4.3	0.000e+00	0.00494	0.422	1.139
hon_000_16020	CdGa ₂ La ₂ Nd ₂	7	-3.788	-4.029	-8.000e-06	0.00597	0.739	0.481
hon_000_16023	Sn ₃ Tb ₂ Zr	6	-4.994	-5.254	-3.400e-05	0.00508	0.503	0.328
hon_000_16029	GaNi ₂ PdY ₂	6	-5.824	-5.892	2.000e-06	0.00837	0.233	0.247
hon_000_16054	Fe ₂ GaLiPtSe ₂	7	-4.68	-4.919	-8.000e-06	0.00697	1.444	2.295
hon_000_16073	Ga ₂ MoRu ₂ Zr	6	-7.283	-7.454	-5.000e-06	0.00702	0.408	1.92
hon_000_16086	CaGaNi ₂ Sb	5	-3.463	-4.43	-4.000e-06	0.00922	1.096	2.447
hon_000_16104	Ga ₂ Ni ₃ Ti	6	-5.28	-5.409	-1.800e-05	0.00811	0.276	0.239
hon_000_16107	Ga ₆ Ru ₂	8	-4.124	-4.659	-4.000e-06	0.00557	0.94	1.979
hon_000_16191	Co ₄ Ge ₂	6	-5.875	-6.169	-2.000e-06	0.00645	0.266	0.336
hon_000_16196	PdRu ₂ Zr ₃	6	-7.93	-8.483	-1.690e-04	0.00767	1.039	1.507
hon_000_16240	BiDy ₂ Eu ₃	6	-3.177	-3.262	-6.000e-06	0.00416	0.558	2.213
hon_000_16252	AlFe ₂ LaSi	5	-5.697	-5.994	0.000e+00	0.00639	0.64	1.381
hon_000_16286	AgMgNa ₃ Ni ₂	7	-2.333	-2.407	-2.000e-06	0.00976	0.335	0.467
hon_000_16295	Fe ₂ GaHf ₂ LiPtSi	8	-6.4	-6.712	0.000e+00	0.00723	0.807	1.64
hon_000_16299	CdGd ₃ IrMgZr	7	-4.744	-4.997	2.000e-06	0.00575	0.614	1.714
hon_000_16356	AcCdNaYb ₂	5	-1.48	-1.854	-1.100e-06	0.00315	1.302	3.806
hon_000_16371	AgRu ₂ Tb ₂ Tl	6	-4.763	-5.496	-2.100e-05	0.00788	0.787	0.476
hon_000_16375	GaNi ₂ YZn	5	-4.224	-4.7	5.000e-06	0.00811	1.132	2.323
hon_000_16388	Rh ₂ Sn ₄ Tb ₂	8	-5.064	-5.402	-2.000e-06	0.00833	0.443	2.719
hon_000_16393	Dy ₃ Sn ₃	6	-4.559	-4.801	0.000e+00	0.00926	1.159	1.052
hon_000_16398	Gd ₂ Pd ₂ Sn ₄	8	-4.688	-4.87	-1.000e-06	0.00367	0.72	0.643
hon_000_16414	Ni ₃ Te ₃	6	-3.946	-4.33	-5.000e-05	0.00794	1.295	0.633
hon_000_16421	Mn ₂ PdSn ₅	8	-4.032	-5.124	8.000e-06	0.00386	0.908	1.681
hon_000_16426	Br ₆ Gd ₂	8	-3.982	-4.285	-7.000e-06	0.00481	0.718	2.08
hon_000_16449	AlGaNi ₂ Sn ₂ Yb	7	-3.853	-4.133	-1.000e-06	0.00705	1.097	1.87
hon_000_16479	CdYb ₅	6	-1.335	-1.425	-3.700e-06	0.00241	1.361	1.881
hon_000_16517	Sn ₄ Yb ₂	6	-3.181	-3.456	-1.000e-05	0.00531	0.857	1.449
hon_000_16532	NaSn ₂ Tb ₃	6	-3.633	-4.165	-4.000e-06	0.00365	1.106	1.929
hon_000_16557	Ir ₂ Nd ₂ Rb ₂ Te ₂	8	-4.452	-4.812	0.000e+00	0.0085	1.87	2.122
hon_000_16561	Gd ₂ MgSn ₃	6	-3.914	-4.22	0.000e+00	0.00427	1.623	2.473
hon_000_16581	GaHg ₂ HoNd ₂	6	-2.855	-3.231	-5.000e-06	0.00737	0.724	2.63
hon_000_16587	AlPdRu ₂ Y	5	-6.707	-6.971	-2.300e-05	0.00674	0.438	0.272
hon_000_16589	Co ₃ GeLa ₂	6	-6.05	-6.164	0.000e+00	0.00824	0.333	0.236
hon_000_16622	Co ₂ Ga ₄	6	-3.93	-4.33	0.000e+00	0.00436	0.737	2.527
hon_000_16673	Cl ₄ Tb ₂ Zr ₂	8	-4.494	-5.193	-1.100e-05	0.00866	1.257	2.997
hon_000_16714	Sn ₂ Tb ₂ ThTm	6	-5.041	-5.088	-7.000e-06	0.00846	0.209	1.345
hon_000_16720	Cd ₃ MgTb ₂	6	-2.061	-2.303	-6.000e-06	0.00275	0.57	2.432
hon_000_16721	Co ₂ La ₂ SiZn	6	-5.22	-5.371	-2.000e-06	0.00561	0.435	0.378
hon_000_16752	Co ₄ Ge ₂	6	-6.115	-6.172	3.000e-06	0.00825	0.173	1.538
hon_000_16772	MgNdPrSrTb ₂	6	-3.431	-3.482	6.000e-06	0.0084	0.235	0.198
hon_000_16781	Dy ₃ Sn ₃	6	-4.439	-4.794	-3.000e-06	0.00642	0.892	1.646
hon_000_16793	Br ₄ PtYb ₂	7	-2.776	-3.743	0.000e+00	0.00679	1.639	3.415
hon_000_16839	Dy ₄ GaSb	6	-4.4	-4.63	-7.000e-06	0.00263	0.657	0.748
hon_000_16848	Ga ₂ Mn ₂ Mo ₂	6	-7.322	-7.448	-1.000e-06	0.00898	0.23	0.244
hon_000_16871	Ga ₂ Ni ₂ ScSi	6	-4.596	-5.193	0.000e+00	0.00965	0.642	2.49
hon_000_16886	AlMgMn ₂ OsPt	6	-6.552	-6.723	0.000e+00	0.00677	0.728	0.538
hon_000_16887	Dy ₂ Ga ₆	8	-3.377	-3.736	-1.000e-06	0.00928	0.663	1.561

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_16909	Ga ₅ Gd ₃	8	-3.489	-4.117	0.000e+00	0.00588	1.459	2.031
hon_000_16915	Cl ₄ Nd ₂ Pt	7	-3.681	-4.684	-1.900e-05	0.00781	1.537	2.895
hon_000_16983	Gd ₂ I ₄ Pd	7	-3.161	-3.752	-3.000e-06	0.00555	2.202	2.965
hon_000_16994	GaRu ₂ Sm ₂	5	-5.987	-6.271	7.000e-06	0.0036	0.658	1.493
hon_000_16997	AlGdGe ₂ Mn ₂	6	-5.205	-5.907	0.000e+00	0.00486	0.984	1.338
hon_000_17007	CrFeMn ₂ Si ₂	6	-7.776	-7.911	-2.000e-06	0.00774	0.214	1.08
hon_000_17012	Ru ₂ Zr ₄	6	-8.575	-8.897	-1.000e-06	0.00308	0.727	1.354
hon_000_17019	Gd ₂ Na ₂ S ₂ W ₂	8	-5.394	-5.846	-3.000e-06	0.00591	1.798	2.244
hon_000_17033	CdMg ₂ Yb ₃	6	-1.301	-1.456	-3.000e-07	0.00489	1.45	3.083
hon_000_17038	MoNi ₃ Ti ₂	6	-7.055	-7.326	-1.000e-06	0.00944	0.164	0.959
hon_000_17061	Cl ₄ Ir ₂ Tb ₂	8	-4.472	-5.324	-1.000e-06	0.00592	1.704	2.206
hon_000_17065	MgNd ₂ Sn ₃	6	-3.891	-4.266	0.000e+00	0.00245	1.491	1.109
hon_000_17080	Cl ₃ PdTb ₂	6	-3.736	-4.818	-1.800e-05	0.0045	1.873	1.47
hon_000_17083	Cl ₄ Nd ₂ Pt	7	-3.917	-4.693	-7.000e-06	0.00459	0.901	0.966
hon_000_17098	HAlDyFe ₂ Si	6	-4.974	-5.756	0.000e+00	0.00742	0.559	1.83
hon_000_17099	Dy ₂ Sn ₄	6	-3.964	-4.62	-1.000e-06	0.01	1.715	1.97
hon_000_17112	Ru ₂ Se ₆	8	-4.77	-5.123	-2.000e-06	0.00449	0.501	0.636
hon_000_17121	Al ₄ Mg ₂ Ru ₂	8	-4.426	-4.619	-1.000e-05	0.00548	0.442	1.069
hon_000_17126	K ₃ NaYb ₂	6	-1.002	-1.074	-9.000e-07	0.00356	0.447	0.759
hon_000_17153	Cs ₄ Dy ₂	6	-1.374	-1.474	-5.600e-06	0.00693	1.875	4.637
hon_000_17175	AgAlCaSb ₂ Yb ₂	7	-2.86	-3.363	0.000e+00	0.00387	1.292	1.611
hon_000_17184	Al ₃ LiRu ₂	6	-5.129	-5.553	-1.000e-05	0.00846	0.985	2.075
hon_000_17188	Ni ₂ Sn ₄ Tb ₂	8	-4.584	-4.837	0.000e+00	0.00995	1.543	1.921
hon_000_17189	Ge ₂ Mn ₂ Pd ₂	6	-6.034	-6.24	-1.000e-06	0.00673	0.655	1.674
hon_000_17206	AlNi ₂ Ru ₃ TbTm	8	-6.234	-6.677	6.000e-06	0.00796	0.573	1.151
hon_000_17218	AlFeMn ₂ Si ₂	6	-6.797	-6.919	-1.000e-06	0.00535	0.23	0.321
hon_000_17234	Cl ₄ Dy ₂ Ir ₂	8	-4.425	-5.256	3.000e-06	0.00951	0.609	1.225
hon_000_17238	Cs ₄ Yb ₂	6	-0.679	-0.855	-1.200e-06	0.00197	1.01	2.02
hon_000_17248	Co ₃ GaNdPd	6	-5.629	-5.766	0.000e+00	0.00771	0.324	0.869
hon_000_17251	Ru ₂ Zr ₄	6	-8.352	-8.86	-5.000e-06	0.00798	0.653	0.49
hon_000_17264	AlCrMgRu ₂ Si ₃	8	-6.142	-6.255	-4.000e-06	0.00285	0.261	0.845
hon_000_17305	Cd ₂ Gd ₂ Nd ₂	6	-3.188	-3.437	0.000e+00	0.00809	0.596	0.398
hon_000_17313	AlFe ₃ Tm ₂	6	-5.966	-6.191	-1.000e-06	0.0041	0.659	1.197
hon_000_17317	Al ₃ PtRu ₂	6	-6.432	-6.452	-2.000e-06	0.00437	0.088	0.112
hon_000_17322	Ni ₂ PdTiU	5	-6.815	-7.135	-2.000e-05	0.00673	0.629	1.32
hon_000_17338	AlCo ₄ Dy ₂	7	-5.763	-5.884	-1.220e-04	0.00772	0.501	1.573
hon_000_17342	GeMn ₂ Zn ₃	6	-3.977	-4.138	0.000e+00	0.00775	0.401	1.754
hon_000_17361	AlAuRu ₂ Y ₂	6	-6.631	-6.781	-9.000e-06	0.00671	0.414	1.9
hon_000_17363	Ga ₂ Na ₂ Pd ₂ Tb ₂	8	-3.504	-3.825	0.000e+00	0.00337	1.311	1.486
hon_000_17408	Li ₂ Ni ₂ SnZn	6	-3.259	-3.802	-2.000e-06	0.00788	1.729	2.124
hon_000_17502	Dy ₂ Nd ₂ Pb ₂	6	-4.401	-4.58	6.000e-06	0.00467	0.414	0.413
hon_000_17520	Ni ₅ Sb	6	-5.196	-5.335	-3.000e-06	0.00703	0.69	1.941
hon_000_17524	Mg ₂ Nd ₂ Sn ₂	6	-3.534	-3.785	0.000e+00	0.00462	1.46	3.133
hon_000_17531	HoLiMgNd ₃	6	-3.462	-3.664	3.000e-06	0.00226	0.993	0.647
hon_000_17559	GaNi ₄ Ti	6	-5.491	-5.789	-4.900e-05	0.008	0.568	1.819
hon_000_17584	Al ₃ Fe ₂ Si	6	-5.411	-5.674	-1.400e-05	0.00434	0.922	1.485
hon_000_17601	Nd ₂ Sn ₄	6	-4.436	-4.671	0.000e+00	0.00743	1.353	0.724
hon_000_17604	Gd ₂ Sn ₃ Tl	6	-3.84	-4.164	2.000e-06	0.0083	0.582	1.917
hon_000_17610	MgSn ₂ Yb ₃	6	-2.347	-2.695	0.000e+00	0.00301	1.255	1.8
hon_000_17611	AlNi ₂ Pt ₃	6	-5.555	-5.848	1.000e-06	0.0074	0.359	0.937
hon_000_17612	Ca ₂ MgSnYb ₂	6	-2.075	-2.264	-6.000e-06	0.00147	1.174	1.992
hon_000_17617	Dy ₂ Gd ₄	6	-4.519	-4.561	8.000e-06	0.00275	0.184	0.148

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_17635	Nd ₂ Te ₃	5	-4.235	-5.123	-1.000e-06	0.00325	2.553	2.83
hon_000_17666	Nd ₃ Sn ₂	5	-4.427	-4.945	-5.000e-06	0.00654	0.831	2.234
hon_000_17707	Cl ₄ Gd ₂ U	7	-4.334	-5.023	5.000e-06	0.00413	2.138	1.974
hon_000_17712	In ₄ Yb ₂	6	-2.292	-2.572	-3.000e-06	0.00698	1.507	1.895
hon_000_17743	GdLiNi ₂ SiZn	6	-4.037	-4.298	4.000e-06	0.00676	0.542	2.01
hon_000_17769	Au ₄ Fe ₂	6	-3.77	-4.538	0.000e+00	0.00385	1.356	1.777
hon_000_17774	Dy ₆	6	-4.509	-4.522	3.000e-06	0.00434	0.124	0.085
hon_000_17783	C ₂ GaRu ₂ SmTbW	8	-7.307	-7.752	-3.000e-06	0.00675	1.187	1.174
hon_000_17795	Ga ₄ Ru ₂	6	-4.898	-5.137	1.000e-06	0.00596	0.623	1.149
hon_000_17811	Au ₂ Cu ₃ Dy ₂	7	-3.521	-4.237	-7.000e-06	0.00689	1.388	2.493
hon_000_17818	Sn ₃ Yb ₃	6	-2.914	-3.157	-1.000e-06	0.00469	0.83	0.501
hon_000_17821	Cl ₄ Ir ₂ Nd ₂	8	-4.607	-5.323	-1.000e-06	0.00606	1.68	2.207
hon_000_17860	Ga ₂ Mn ₂ Si ₂	6	-5.298	-5.671	-3.000e-06	0.0058	0.745	0.863
hon_000_17872	GaNd ₂ Ru ₂ Tl	6	-4.997	-5.666	-5.000e-06	0.0038	1.382	3.809
hon_000_17906	Fe ₂ Se ₄	6	-4.423	-5.15	0.000e+00	0.00277	1.155	1.921
hon_000_17908	GaNi ₂ Th ₂	5	-3.756	-6.049	-4.100e-05	0.0089	1.164	2.551
hon_000_17944	ErGaRu ₂ Y	5	-5.777	-6.648	1.000e-06	0.00769	0.99	1.197
hon_000_17947	Fe ₂ Te ₄ Yb ₂	8	-4.059	-4.536	-2.400e-05	0.00375	1.431	2.544
hon_000_17951	Al ₄ Fe ₂	6	-5.012	-5.379	-8.100e-05	0.00382	0.451	1.157
hon_000_17954	Br ₆ Nd ₂	8	-4.132	-4.307	-7.000e-06	0.00429	0.665	1.34
hon_000_17978	Cd ₃ Ru ₂	5	-3.493	-3.78	-2.000e-06	0.00525	0.459	0.236
hon_000_17981	AlGePd ₂ Ru ₂	6	-6.295	-6.395	-6.000e-06	0.00741	0.282	1.722
hon_000_17987	Ga ₂ Ru ₂ Zr ₂	6	-6.913	-7.23	-2.300e-05	0.00693	0.852	0.522
hon_000_18027	Sn ₃ Yb ₂	5	-2.824	-3.382	-1.000e-06	0.00441	1.603	1.183
hon_000_18072	Co ₂ Li ₂ MnSn ₃	8	-4.6	-4.669	-1.000e-05	0.00735	0.28	0.831
hon_000_18076	PdPtRu ₂ SnTi	6	-7.104	-7.191	0.000e+00	0.00892	0.184	1.722
hon_000_18084	INd ₂ Sn ₂ Sr	6	-3.575	-3.944	-1.000e-06	0.00354	0.948	2.602
hon_000_18092	GaMgTl ₂ Yb ₂	6	-1.912	-2.178	-2.000e-06	0.00346	0.921	1.327
hon_000_18102	Br ₆ Yb ₂	8	-2.902	-3.129	-2.500e-05	0.00876	1.349	3.527
hon_000_18103	Gd ₄ InMg	6	-3.772	-3.831	0.000e+00	0.00297	0.383	0.465
hon_000_18110	Br ₄ Nd ₂ Pt ₂	8	-3.887	-4.608	-5.000e-06	0.00687	0.78	2.35
hon_000_18113	Ga ₃ Ru ₂ Tb ₃	8	-5.249	-5.513	-2.000e-06	0.00914	0.666	1.467
hon_000_18129	Cd ₄ Co ₂	6	-2.158	-2.495	0.000e+00	0.00734	1.23	1.806
hon_000_18146	Gd ₄ Hg ₂ Sr	7	-2.876	-3.039	0.000e+00	0.00203	0.89	1.636
hon_000_18214	Co ₄ CuLa	6	-5.639	-5.898	-2.500e-05	0.00946	0.707	1.307
hon_000_18223	Gd ₂ Sn ₄	6	-4.316	-4.496	-4.000e-06	0.00369	0.227	1.462
hon_000_18295	AuGeNi ₂ SnV	6	-5.153	-5.322	-2.000e-06	0.00549	0.768	1.391
hon_000_18314	CuGaRu ₂ U ₂	6	26.537	-7.924	-1.000e-06	0.00762	0.405	1.188
hon_000_18324	Li ₂ Ni ₂ Sn	5	-3.607	-3.734	-2.000e-06	0.00575	0.356	2.155
hon_000_18331	Mg ₃ Nd ₃	6	-3.007	-3.15	-2.000e-06	0.00271	0.942	1.778
hon_000_18361	Co ₂ Gd ₂ SnZn	6	-4.607	-4.939	2.000e-06	0.00746	0.945	0.837
hon_000_18374	Ga ₃ Ni ₂	5	-4.001	-4.131	-2.900e-05	0.00784	0.403	0.368
hon_000_18381	Fe ₂ Li ₃ P	6	-4.284	-4.607	-1.200e-05	0.00633	0.545	1.831
hon_000_18438	Cl ₄ Dy ₂ W	7	-4.375	-5.063	1.000e-06	0.00859	1.175	1.914
hon_000_18454	AlBeLiNi ₂ Zn	6	-3.654	-3.789	0.000e+00	0.00947	0.583	1.956
hon_000_18463	Fe ₂ GePtSi	5	-6.069	-6.635	-5.000e-06	0.00959	0.399	1.031
hon_000_18469	As ₂ CuNi ₃ Sm	7	-4.988	-5.286	3.000e-06	0.00948	0.747	1.463
hon_000_18472	Al ₂ Ga ₂ Ru ₂	6	-5.442	-5.488	-1.000e-06	0.00595	0.24	0.895
hon_000_18500	DyGd ₃ Li ₂	6	-3.324	-3.606	-5.000e-06	0.00489	1.006	0.837
hon_000_18501	SnTb ₂ Te ₂	5	-3.71	-4.688	0.000e+00	0.00324	1.68	1.988
hon_000_18512	Sn ₄ Yb ₂	6	-3.277	-3.462	2.000e-06	0.00843	0.67	1.427
hon_000_18546	Al ₃ Fe ₂ Hf ₂ P	8	-6.569	-7.002	-2.620e-04	0.00704	1.01	1.884

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_18548	Co ₃ Ga ₂ Pt	6	-5.535	-5.568	0.000e+00	0.008	0.147	0.175
hon_000_18567	CdTe ₃ Yb ₂	6	-2.648	-3.345	-3.000e-06	0.00892	1.603	3.254
hon_000_18591	Cl ₆ Nd ₂	8	-4.711	-4.822	-1.000e-05	0.00832	0.515	0.352
hon_000_18601	AlFe ₂ GaPd ₂	6	-5.632	-5.707	-2.000e-06	0.00509	0.13	0.863
hon_000_18642	Al ₂ Er ₃ Fe ₂	7	-5.033	-5.486	-1.000e-06	0.00811	0.934	1.575
hon_000_18666	AlGeNi ₃	5	-5.14	-5.178	-3.000e-06	0.00722	0.215	1.009
hon_000_18675	AuGa ₂ LiRu ₂	6	-4.953	-5.021	-3.000e-06	0.00659	0.165	1.007
hon_000_18682	AsDy ₂ GaSe ₃	7	-4.077	-4.933	0.000e+00	0.00349	1.276	2.229
hon_000_18702	Tb ₂ Tl ₄	6	-2.797	-3.175	-2.000e-05	0.00687	1.372	0.929
hon_000_18713	C ₂ LiPdRu ₂ ScY	8	-6.814	-7.282	-9.000e-06	0.00743	1.045	1.299
hon_000_18724	Fe ₃ Li ₃	6	-4.498	-4.666	-8.000e-06	0.00392	0.351	0.444
hon_000_18730	Na ₃ Nd ₂ Tl	6	-2.508	-2.547	-5.000e-06	0.00577	0.275	0.229
hon_000_18743	AlNi ₂ Pt ₂	5	-5.352	-5.651	-2.000e-06	0.00841	0.173	1.166
hon_000_18752	Li ₄ Ni ₂ Sb	7	-3.25	-3.339	0.000e+00	0.00933	0.313	0.867
hon_000_18770	Gd ₂ LiMgSn ₂	6	-3.45	-3.701	5.000e-06	0.00594	0.494	2.418
hon_000_18801	Al ₄ Yb ₄	8	-2.367	-2.837	0.000e+00	0.00303	2.177	1.298
hon_000_18820	Ga ₂ Ni ₂ U ₂	6	-6.325	-6.648	-6.000e-06	0.00699	0.5	1.13
hon_000_18836	Dy ₂ Gd ₂ LaSn	6	-4.609	-4.71	-1.000e-06	0.00729	0.34	0.323
hon_000_18886	Cs ₃ Nd ₂	5	-1.705	-1.757	1.800e-06	0.00338	1.38	3.497
hon_000_18894	BaCdGa ₂ Gd ₂	6	-2.848	-3.203	-1.000e-06	0.00644	1.054	2.895
hon_000_18911	Dy ₂ RhSb ₂	5	-5.011	-5.75	-2.000e-06	0.00568	1.475	1.902
hon_000_18918	AsCo ₂ Li ₂ Si	6	-4.319	-4.992	-5.000e-06	0.00864	0.552	1.607
hon_000_18968	GaRu ₂ U ₂ Zr	6	-8.486	-8.828	-1.200e-05	0.00447	1.159	1.611
hon_000_18997	MgNd ₂ Sn ₃	6	-3.976	-4.252	-6.000e-06	0.00493	1.466	3.043
hon_000_19003	FeNi ₃ PtSe	6	-5.33	-5.528	0.000e+00	0.00694	0.503	0.523
hon_000_19018	Co ₂ GaPr ₂ Si	6	-5.444	-5.626	0.000e+00	0.00404	0.583	0.667
hon_000_19025	AlRh ₂ SbSnTb ₂ Tl	8	-4.727	-5.193	0.000e+00	0.00465	1.202	1.677
hon_000_19026	Gd ₃ SnSr ₂	6	-3.492	-3.546	-1.000e-06	0.00365	0.239	0.228
hon_000_19037	AuFe ₂ LiSr	5	-4.199	-4.383	-1.300e-05	0.00636	0.341	1.176
hon_000_19060	LiRu ₂ Sn ₃	6	-5.133	-5.323	-1.000e-06	0.00546	1.46	2.523
hon_000_19073	AsCeGeNi ₂	5	-5.195	-5.571	0.000e+00	0.00972	0.34	1.008
hon_000_19121	AsCsCuI ₃ Yb ₂	8	-2.424	-3.051	-2.000e-06	0.00448	1.772	2.378
hon_000_19123	Cs ₃ HgNd ₂	6	-1.468	-1.673	-1.000e-06	0.00267	1.23	2.803
hon_000_19132	CdCeDy ₂ Sb	5	-3.924	-4.41	-1.000e-05	0.00739	1.404	3.992
hon_000_19154	Co ₂ GdSbSn ₂	6	-4.799	-5.285	-1.600e-05	0.00684	0.358	0.816
hon_000_19157	Ni ₂ Zn ₄	6	-2.613	-2.697	1.000e-06	0.00511	0.181	0.122
hon_000_19171	K ₃ Yb ₂	5	-0.866	-0.95	-2.910e-05	0.00368	0.591	1.689
hon_000_19203	Dy ₃ MgSn ₂	6	-4.081	-4.257	-7.000e-06	0.00515	1.918	1.753
hon_000_19208	AuCo ₂ Er ₂ Pd	6	-5.528	-5.627	-4.000e-06	0.00794	0.434	0.451
hon_000_19232	CdMgNi ₃ Sn	6	-3.451	-3.808	-2.700e-05	0.00589	0.499	0.366
hon_000_19235	Al ₂ AuCo ₅	8	-5.417	-5.834	-2.800e-05	0.00661	0.63	1.704
hon_000_19247	GaLu ₂ Ru ₃	6	-6.455	-6.843	-4.000e-06	0.00831	0.34	0.291
hon_000_19286	AuFe ₂ Gd ₂ Si	6	-5.727	-6.007	-1.000e-05	0.00591	0.693	1.371
hon_000_19312	HAfFe ₃ Pr	6	-5.409	-5.966	2.000e-06	0.00755	0.591	0.884
hon_000_19339	Co ₂ MgPrPtZn ₂	7	-4.005	-4.184	1.100e-05	0.00852	0.668	1.284
hon_000_19370	Cl ₄ Rh ₂ Tb ₂	8	-4.178	-5.063	1.000e-06	0.00475	1.6	2.681
hon_000_19398	CdCe ₂ Dy ₂ Tl	6	-3.724	-3.994	-5.000e-06	0.00634	0.54	0.532
hon_000_19399	Ga ₂ PtRu ₂ Si	6	-6.071	-6.267	0.000e+00	0.00496	0.21	0.317
hon_000_19403	GeNi ₂ SiTm	5	-5.043	-5.446	0.000e+00	0.00576	0.676	1.054
hon_000_19422	AgCo ₂ GaLa ₂	6	-5.026	-5.076	3.000e-06	0.00888	0.433	1.179
hon_000_19453	Cl ₄ Nd ₂ W	7	-4.46	-5.161	-3.000e-06	0.00429	1.518	1.237
hon_000_19458	Cs ₄ Yb ₂	6	-0.723	-0.836	5.500e-06	0.00154	0.86	0.536

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_19468	Co ₂ Ga ₂ Tm	5	-4.689	-5.082	0.000e+00	0.00337	0.777	2.145
hon_000_19480	Dy ₂ Sn ₄	6	-4.243	-4.583	-5.000e-06	0.0055	1.846	1.562
hon_000_19526	Ni ₂ SbTb ₂	5	-5.252	-5.427	-2.300e-05	0.00428	0.288	0.123
hon_000_19527	Al ₄ Co ₂ Ni	7	-4.878	-5.161	-4.000e-05	0.0083	0.444	1.077
hon_000_19532	AlAuNa ₃ Nd ₂ Sn	8	-2.825	-3.157	-1.000e-06	0.00638	1.173	1.084
hon_000_19536	GaNi ₂ PdTiZr	6	-5.964	-6.181	-4.000e-06	0.0059	0.775	1.494
hon_000_19540	Co ₄ Li ₂ Ti	7	-5.094	-5.371	-4.000e-06	0.00757	0.49	0.313
hon_000_19553	Gd ₆	6	-4.569	-4.58	-3.000e-06	0.00341	0.119	0.069
hon_000_19556	AlCuNi ₂ Y ₂	6	-5.468	-5.582	-2.200e-05	0.00712	0.452	1.716
hon_000_19563	Mn ₂ Sn ₃	5	-4.916	-5.468	-5.000e-06	0.00858	0.653	2.364
hon_000_19595	Dy ₂ Na ₄	6	-2.001	-2.046	-2.000e-06	0.00313	0.336	0.336
hon_000_19612	GeLi ₃ Ni ₂	6	-3.557	-3.75	1.000e-06	0.00315	0.962	1.394
hon_000_19631	Cs ₅ SbTb ₂	8	-1.846	-1.918	6.000e-06	0.00409	0.95	1.113
hon_000_19634	Al ₂ Co ₂ GeLiSc	7	-4.812	-4.989	-1.000e-06	0.00655	0.221	2.452
hon_000_19642	C ₂ Co ₃ Na ₃	8	-4.741	-4.945	-9.000e-06	0.00913	0.499	1.148
hon_000_19643	Ga ₂ LaNi ₂	5	-4.385	-4.752	-2.000e-06	0.0095	1.731	2.426
hon_000_19655	Dy ₂ Sb ₂ Zr	5	-5.011	-5.638	-3.000e-06	0.00382	1.82	1.455
hon_000_19672	Fe ₂ Ni ₂ Se ₂	6	-5.374	-5.578	-8.000e-06	0.00841	0.861	1.331
hon_000_19675	Dy ₂ Gd ₂ Y ₂	6	-5.05	-5.169	-2.000e-06	0.00181	0.628	1.639
hon_000_19693	AlFeMn ₂ Sb ₃	7	-5.432	-5.802	0.000e+00	0.00854	1.1	1.576
hon_000_19703	Co ₃ HfNa ₂	6	-4.913	-5.254	-1.500e-05	0.00812	0.912	2.674
hon_000_19721	Gd ₄ MgSn	6	-3.957	-4.185	-2.000e-06	0.00225	1.654	0.985
hon_000_19725	Gd ₂ S ₆	8	-4.423	-5.25	-1.000e-06	0.00456	3.165	3.015
hon_000_19726	H ₄ BMn ₂	7	-4.571	-5.16	0.000e+00	0.00278	0.848	0.817
hon_000_19750	GeNi ₃ V ₂	6	-6.691	-6.779	-2.200e-05	0.00911	0.202	0.913
hon_000_19751	CrFe ₂ GaLi ₂	6	-4.897	-5.341	1.000e-06	0.00826	0.407	0.807
hon_000_19765	K ₂ Sr ₂ Tb ₂	6	-1.902	-2.021	2.000e-06	0.00485	0.861	3.947
hon_000_19809	AsLaMnNi ₂	5	-5.694	-6.189	-1.000e-06	0.00832	0.59	1.836
hon_000_19813	Ga ₃ LiNi ₂	6	-3.732	-3.816	-1.000e-06	0.00696	0.265	1.654
hon_000_19847	Ga ₄ Ni ₂	6	-3.611	-3.913	-1.000e-06	0.00416	0.632	2.537
hon_000_19887	Cl ₃ Gd ₂ Pd	6	-3.626	-4.792	0.000e+00	0.00504	2.292	2.936
hon_000_19920	Na ₃ ScTb ₂	6	-2.801	-2.823	-2.000e-06	0.00551	0.135	2.243
hon_000_19934	BrCl ₃ IrTb ₂	7	-3.901	-4.941	-2.000e-06	0.00845	1.864	4.419
hon_000_19955	Ca ₂ Ru ₂ Si	5	-4.781	-5.471	0.000e+00	0.00398	1.392	1.814
hon_000_19977	Co ₅ Er ₂ Ga	8	-5.659	-5.816	-2.000e-06	0.00831	0.583	0.516
hon_000_19980	Dy ₃ Sn ₂	5	-4.298	-4.592	2.000e-06	0.00317	1.401	1.006
hon_000_19997	CrNi ₂ Si ₃	6	-6.23	-6.455	-4.000e-05	0.00683	0.486	1.266
hon_000_20009	AuNi ₂ PtSi ₂	6	-4.938	-5.462	1.000e-06	0.00918	0.507	1.284
hon_000_20029	PRu ₂ Sn ₂ Sr ₂ Zn	8	-4.156	-4.797	0.000e+00	0.0078	0.798	1.721
hon_000_20097	Gd ₄ LuSn	6	-4.518	-4.663	0.000e+00	0.00464	0.882	0.55
hon_000_20098	Cl ₄ IrTb ₂	7	-4.024	-5.003	0.000e+00	0.00396	1.073	1.712
hon_000_20108	DySn ₂ Tb ₃	6	-4.343	-4.671	-2.000e-05	0.00442	0.801	0.391
hon_000_20137	Al ₂ Fe ₂ Sc ₂ Si	7	-5.8	-6.025	2.000e-06	0.00666	1.213	2.438
hon_000_20176	IrLiNi ₂ Tb ₃	7	-5.074	-5.338	-1.200e-05	0.00849	0.966	2.208
hon_000_20200	Au ₂ Br ₃ ClNd ₂	8	-3.174	-4.105	-2.000e-06	0.00414	2.003	1.745
hon_000_20217	Cl ₄ Nd ₂ Ru ₂	8	-4.516	-5.323	2.000e-06	0.00968	1.482	2.615
hon_000_20221	PrSnTb ₄	6	-4.629	-4.679	0.000e+00	0.00425	0.244	1.204
hon_000_20233	Ag ₂ Fe ₂ Li ₂ P ₂	8	-4.394	-4.558	-3.300e-05	0.00586	0.473	0.865
hon_000_20272	Dy ₂ Se ₃ Si ₂ Te	8	-4.299	-4.987	-1.000e-06	0.0043	1.741	1.656
hon_000_20273	CaDy ₂ LiMg ₂	6	-2.522	-2.609	-1.000e-06	0.00199	0.806	0.513
hon_000_20285	Cs ₃ Dy ₂	5	-1.336	-1.891	-1.000e-05	0.00466	2.998	4.17
hon_000_20295	Gd ₂ Mg ₂ SnZr	6	-4.002	-4.278	-4.000e-06	0.00393	1.522	0.826

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_20300	Fe ₂ La ₂ Te	5	-6.155	-6.368	-1.000e-06	0.0027	0.507	2.311
hon_000_20365	AlCo ₅	6	-6.355	-6.514	-1.000e-05	0.00807	0.372	0.309
hon_000_20378	Fe ₂ Ga ₂ LiNa	6	-3.528	-4.102	-2.000e-06	0.00672	0.382	2.239
hon_000_20389	Al ₂ GeNd ₃ RuSe	8	-4.907	-5.41	0.000e+00	0.00643	1.205	2.695
hon_000_20394	Al ₅ Mn ₃	8	-5.41	-5.787	-4.000e-06	0.0092	0.864	0.578
hon_000_20409	GeNi ₂ Sc ₂ Zn	6	-5.118	-5.243	-1.500e-05	0.0089	0.433	1.841
hon_000_20418	CsK ₃ Tb ₂	6	-1.464	-1.726	-1.300e-05	0.0056	2.989	4.676
hon_000_20488	Cl ₄ Gd ₂ Sn	7	-3.385	-4.446	0.000e+00	0.00457	1.451	2.783
hon_000_20504	GdLuNd ₂ Sn ₂	6	-4.253	-4.803	-2.000e-06	0.00768	1.365	1.759
hon_000_20514	Cl ₄ PdTb ₂	7	-3.669	-4.803	0.000e+00	0.00467	2.073	2.382
hon_000_20550	AlAs ₂ KPbTb ₂	7	-3.862	-4.286	-2.000e-06	0.0037	1.083	0.682
hon_000_20551	AlCaLaTb ₃	6	-3.904	-4.023	-1.000e-06	0.00384	0.39	1.437
hon_000_20568	Pt ₂ Ru ₂ Sc	5	-7.572	-7.69	-1.700e-05	0.00895	0.687	1.418
hon_000_20571	Cl ₆ Ru ₂	8	-4.151	-4.192	-1.300e-05	0.00673	0.439	0.439
hon_000_20621	Nd ₂ Se ₄ W	7	-5.281	-6.285	-1.000e-06	0.00361	1.832	1.573
hon_000_20656	DyGaNi ₂ Y	5	-4.788	-5.401	-2.000e-06	0.00694	1.255	1.718
hon_000_20697	Cd ₂ Ga ₂ Gd ₂ Nd ₂	8	-3.338	-3.583	0.000e+00	0.00343	0.879	0.798
hon_000_20710	AgAsNd ₂ Ru ₂	6	-5.5	-6.256	-2.000e-06	0.00624	0.916	1.579
hon_000_20715	Ru ₂ SnY ₂	5	-7.028	-7.291	-1.300e-05	0.00699	0.723	0.714
hon_000_20749	Cs ₄ Yb ₂	6	-0.721	-0.856	6.000e-07	0.00281	0.82	2.847
hon_000_20786	Gd ₂ Pt ₂ Sn ₂	6	-5.349	-5.565	-4.000e-06	0.00601	0.897	0.496
hon_000_20789	LiNi ₃ Sn	5	-4.231	-4.504	-1.000e-06	0.00531	0.395	2.128
hon_000_20790	Au ₃ Fe ₂	5	-4.536	-4.735	3.000e-06	0.00488	0.398	1.132
hon_000_20804	Co ₂ SSrV	5	-5.627	-5.988	0.000e+00	0.00762	0.787	2.005
hon_000_20838	Ni ₃ Si ₃	6	-5.583	-5.756	-1.000e-06	0.00427	0.503	0.472
hon_000_20878	GeLi ₂ Ru ₂ Si	6	-5.159	-5.736	-7.000e-06	0.00556	0.492	1.532
hon_000_20924	Fe ₂ Zn ₂ Zr ₂	6	-5.646	-6.032	7.000e-06	0.00855	1.369	2.652
hon_000_20929	CdDy ₂ GaNa ₂	6	-2.371	-2.597	0.000e+00	0.00712	0.937	0.703
hon_000_20931	CdDy ₃ NdTl	6	-3.454	-3.764	-2.000e-06	0.00608	1.189	1.98
hon_000_20951	Co ₂ GePt ₃	6	-5.81	-6.116	-3.000e-06	0.00505	0.679	2.163
hon_000_20966	Nd ₂ Se ₄ Ti ₂	8	-5.29	-6.091	-5.000e-06	0.00334	1.855	1.633
hon_000_20970	Co ₃ GeSi ₂ Ti ₂	8	-6.35	-7.087	-1.000e-05	0.00783	0.649	0.673
hon_000_20999	Tl ₃ Yb ₃	6	-1.99	-2.282	3.000e-06	0.00374	1.615	1.234
hon_000_21013	SnTb ₂ Tl ₂ Zr	6	-4.189	-4.526	-3.000e-06	0.00261	0.717	0.37
hon_000_21040	Dy ₃ Mg ₂ Y	6	-3.773	-3.884	-2.000e-06	0.002	0.828	2.567
hon_000_21071	CoMn ₂ Sn ₂	5	-5.479	-6.205	-2.500e-05	0.00728	0.967	0.935
hon_000_21096	Cs ₂ RbYb ₂	5	-0.842	-0.875	-5.000e-07	0.0016	0.476	0.731
hon_000_21098	Al ₃ AuGaRu ₂ Tb	8	-5.065	-5.412	-2.000e-06	0.00494	0.653	1.641
hon_000_21104	Gd ₄ SrY	6	-4.222	-4.287	0.000e+00	0.00291	0.388	1.537
hon_000_21125	Ge ₂ MgMnNi ₂	6	-4.78	-5.1	-1.000e-05	0.00893	0.595	1.354
hon_000_21154	Cs ₂ Sr ₂ Yb ₂	6	-0.906	-1.093	2.700e-06	0.00182	1.214	1.714
hon_000_21173	Cs ₃ RbYb ₂	6	-0.805	-0.866	-2.000e-06	0.00206	0.622	0.4
hon_000_21177	Co ₃ GaTb ₂	6	-5.62	-5.761	-3.000e-06	0.00434	0.403	1.146
hon_000_21179	Al ₂ KSe ₂ Tb ₂ Tl	8	-3.274	-3.844	0.000e+00	0.00306	0.946	3.169
hon_000_21182	Gd ₂ ISnY	5	-4.097	-4.657	0.000e+00	0.00503	1.487	1.366
hon_000_21185	PdRu ₂ U ₂ Zn	6	-7.77	-7.939	2.000e-06	0.00354	0.375	1.087
hon_000_21192	Fe ₂ Gd ₂ Pd	5	-5.892	-6.216	-1.000e-05	0.00845	0.845	1.58
hon_000_21205	CaLaPt ₂ Ru ₂ Sn	7	-5.904	-6.213	-1.400e-05	0.00425	0.348	1.616
hon_000_21207	Co ₂ Ni ₂ SnZn	6	-4.66	-4.903	0.000e+00	0.00748	1.059	0.657
hon_000_21226	Cl ₄ Gd ₂ Pd	7	-3.678	-4.575	-1.000e-06	0.00454	1.484	1.532
hon_000_21266	Co ₃ Mn ₂ Si	6	-7.215	-7.536	-3.000e-06	0.00436	0.254	1.692
hon_000_21281	AuErGaRu ₂ Ti	6	-5.976	-6.541	0.000e+00	0.00519	0.788	0.723

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_21295	Au ₄ LiNi ₂ Sn	8	-3.639	-3.75	1.000e-06	0.00897	0.658	2.276
hon_000_21299	GeRu ₂ SSbSn ₂	7	-5.014	-5.532	1.000e-06	0.00235	0.957	0.964
hon_000_21306	DyTb ₂ Tl ₃	6	-3.389	-3.63	0.000e+00	0.00206	1.022	2.547
hon_000_21315	AlGe ₂ Li ₂ Mn ₃	8	-5.067	-5.402	0.000e+00	0.00602	0.631	1.562
hon_000_21339	AsFe ₂ Rh ₃	6	-6.875	-7.079	-3.000e-06	0.00616	0.425	1.191
hon_000_21341	NaNd ₃ Sn	5	-3.687	-3.893	-1.000e-06	0.00379	1.246	2.182
hon_000_21344	AuFe ₂ Li ₂ V	6	-5.097	-5.288	-3.000e-06	0.00498	0.496	0.323
hon_000_21359	AuFe ₃ PtSbSi ₂	8	-5.829	-6.018	-1.400e-05	0.00452	0.524	1.032
hon_000_21410	Nd ₂ PrSn ₃	6	-4.387	-4.941	-1.000e-05	0.00488	0.894	1.647
hon_000_21420	Al ₂ Fe ₃ Ti	6	-6.326	-6.916	-1.000e-06	0.00364	0.777	1.399
hon_000_21437	CoNi ₅	6	-5.569	-5.601	1.000e-06	0.00621	0.098	0.07
hon_000_21466	Co ₄ Ge ₂	6	-5.837	-6.166	2.000e-06	0.00376	0.255	1.054
hon_000_21468	AlBiRu ₂ Sn	5	-5.59	-5.816	-1.300e-05	0.00687	0.637	0.622
hon_000_21470	Cs ₂ KRbYb ₂	6	-0.848	-0.923	-2.310e-05	0.00296	0.652	1.724
hon_000_21488	LiMgNd ₂ SnTe	6	-3.515	-3.726	-1.000e-06	0.00659	0.559	0.712
hon_000_21490	CoGaNi ₃ Pt	6	-5.39	-5.493	4.000e-06	0.00732	0.292	1.79
hon_000_21515	Al ₃ CoRu ₂	6	-5.94	-6.476	-4.700e-05	0.0062	0.937	2.115
hon_000_21556	GeRu ₂ Sc ₃	6	-7.001	-7.261	-1.000e-06	0.00315	0.702	0.8
hon_000_21574	Pd ₄ Ru ₂	6	-5.807	-6.391	-4.000e-06	0.00735	0.806	0.46
hon_000_21592	AlNi ₄ Pt	6	-5.552	-5.594	-2.700e-05	0.00496	0.152	0.129
hon_000_21594	Co ₂ PtSc ₂ Sn	6	-6.287	-6.43	-1.000e-06	0.00626	0.39	1.046
hon_000_21609	GeLi ₃ Ru ₂	6	-4.509	-4.875	-3.000e-06	0.00901	0.95	1.51
hon_000_21623	Al ₂ Nd ₃ Ru ₂	7	-5.485	-5.98	2.000e-06	0.00667	0.844	1.554
hon_000_21659	Bi ₄ Yb ₂	6	-3.319	-3.57	-2.000e-06	0.00413	1.186	0.788
hon_000_21666	Li ₃ MgNi ₂	6	-2.763	-3.014	-4.000e-06	0.0027	0.857	1.434
hon_000_21678	CuDy ₂ Sb ₂	5	-4.177	-4.953	-2.000e-06	0.00596	1.855	1.141
hon_000_21683	BiFe ₂ Pd ₂	5	-5.641	-5.878	-2.000e-06	0.00451	0.388	0.281
hon_000_21726	Co ₂ Zr ₄	6	-7.733	-8.287	-3.000e-06	0.00813	0.467	1.442
hon_000_21760	Fe ₂ Os ₂ PtSi	6	-7.947	-8.385	-2.000e-06	0.00505	0.269	0.475
hon_000_21762	BeNi ₂ Rh ₂ Si	6	-5.76	-6.173	-1.000e-06	0.00526	1.102	2.133
hon_000_21779	Dy ₂ Pd ₂ S ₄	8	-4.873	-5.825	-1.100e-05	0.00357	1.927	1.434
hon_000_21785	Co ₂ PdSnSr ₂	6	-4.274	-4.449	-3.000e-06	0.00828	0.827	2.345
hon_000_21821	LiMgPdRu ₂ Sn ₂	7	-4.73	-5.061	0.000e+00	0.00617	0.433	1.1
hon_000_21828	Al ₂ Ni ₂ Sm ₂	6	-4.301	-4.889	0.000e+00	0.00975	0.983	1.275
hon_000_21848	Tl ₄ Yb ₂	6	-1.982	-2.24	-1.000e-05	0.00264	0.721	0.758
hon_000_21869	PtRu ₂ Sm ₂ Tl	6	-6.178	-6.278	-2.200e-05	0.00478	0.446	1.888
hon_000_21871	Al ₂ GaMn ₂	5	-5.301	-5.667	-1.000e-06	0.007	0.742	1.463
hon_000_21894	Cs ₄ Dy ₂ Pb ₂	8	-2.244	-2.458	6.000e-06	0.00628	1.396	1.829
hon_000_21916	Ge ₂ LaNi ₂ Rh ₂	7	-5.867	-6.104	0.000e+00	0.00308	1.024	1.542
hon_000_21972	H ₄ Ni ₂	6	-2.83	-3.97	-2.300e-05	0.0058	0.629	1.296
hon_000_21975	Ge ₃ SnTb ₃ Th	8	-4.905	-5.392	-2.000e-06	0.00902	0.292	1.367
hon_000_21992	Gd ₄ LiY	6	-4.314	-4.335	-8.000e-06	0.00392	0.28	0.175
hon_000_22031	Fe ₄ MoPt	6	-8.035	-8.211	-2.000e-06	0.00418	0.188	0.235
hon_000_22036	Ga ₂ PrSbTb ₂	6	-4.141	-4.649	1.000e-06	0.0063	1.05	2.428
hon_000_22048	Gd ₂ PtSe ₄	7	-4.412	-5.496	-1.000e-06	0.00396	1.608	1.765
hon_000_22052	Co ₂ Pt ₆	8	-5.9	-6.141	-6.000e-06	0.00871	0.7	1.65
hon_000_22170	MgSn ₃ Yb ₂	6	-2.795	-3.034	-5.000e-06	0.00972	0.843	0.524
hon_000_22177	Co ₃ Nd ₂ Sn	6	-5.787	-5.826	1.200e-05	0.00724	0.246	0.214
hon_000_22190	Al ₃ Ru ₂ Si	6	-5.925	-6.155	-2.400e-05	0.00447	0.265	1.124
hon_000_22192	HGa ₂ PtRu ₂	6	-5.247	-5.669	-1.000e-06	0.00862	0.358	2.657
hon_000_22200	Ag ₂ Ru ₂ Tb ₂	6	-4.924	-5.463	1.000e-06	0.00732	0.813	0.357
hon_000_22202	AuCo ₂ SiTm	5	-5.175	-5.603	-3.700e-05	0.00518	0.529	1.926

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_22207	PbSnTl ₂ Yb ₂	6	-3.008	-2.789	-1.000e-06	0.00336	0.618	0.39
hon_000_22219	Co ₂ GePtV ₂	6	-7.205	-7.309	1.000e-06	0.00927	0.385	1.126
hon_000_22224	CaTlYb ₄	6	-1.696	-1.793	-2.000e-06	0.00212	1.318	0.86
hon_000_22228	Gd ₂ Tl ₄	6	-3.144	-3.273	-4.000e-06	0.00338	1.204	1.852
hon_000_22245	AuLi ₃ Ru ₂	6	-4.397	-4.569	-3.301e-02	0.00592	0.606	1.147
hon_000_22247	Gd ₂ K ₃ Na	6	-1.691	-1.75	-1.000e-06	0.00377	0.67	0.645
hon_000_22292	Ca ₂ NaTlYb ₂	6	-1.668	-1.83	-2.000e-06	0.00256	1.414	2.632
hon_000_22312	I ₆ Tb ₂	8	-3.644	-3.716	-2.000e-06	0.00785	0.474	2.125
hon_000_22313	Br ₄ Gd ₂ Rh	7	-3.53	-4.551	1.000e-06	0.00732	1.572	4.126
hon_000_22314	Co ₂ Ni ₄	6	-5.722	-5.85	1.000e-06	0.00662	0.575	1.174
hon_000_22317	Ge ₃ MoNi ₂	6	-5.671	-5.969	-2.600e-05	0.00585	0.599	2.136
hon_000_22343	Ga ₃ Ni ₃	6	-4.311	-4.447	-3.000e-06	0.00569	0.551	0.999
hon_000_22355	Ni ₃ Sn ₂	5	-4.8	-4.937	-9.000e-06	0.0087	0.172	1.157
hon_000_22357	AlNi ₂ Pt ₃ Si ₂	8	-5.575	-5.984	0.000e+00	0.00598	0.932	2.463
hon_000_22367	AlBeCo ₂ GeSi	6	-5.164	-5.421	-5.000e-06	0.00722	0.895	1.499
hon_000_22378	GaNd ₂ Ni ₂ Pt	6	-5.492	-5.503	2.000e-06	0.00294	0.094	0.793
hon_000_22380	Fe ₂ Ga ₂ Si ₂	6	-5.079	-5.525	-5.000e-06	0.00437	0.699	1.427
hon_000_22391	Ga ₃ Mn ₃	6	-5.593	-5.881	-6.000e-06	0.0053	1.192	2.143
hon_000_22406	AgAuEu ₃ Ru ₂	7	-4.233	-4.538	0.000e+00	0.00612	1.086	1.522
hon_000_22416	IlrPdSe ₃ Yb ₂	8	-3.944	-4.558	-9.000e-06	0.00415	1.802	1.382
hon_000_22425	Na ₂ Nd ₂ Sn ₂	6	-3.398	-3.55	3.000e-06	0.00497	0.721	0.533
hon_000_22437	EuSn ₃ Yb ₂	6	-2.97	-3.337	0.000e+00	0.00802	1.277	1.769
hon_000_22445	Cl ₃ Gd ₂ Pd	6	-3.661	-4.772	-2.000e-06	0.00445	1.663	2.978
hon_000_22457	Cl ₄ Gd ₂ Pd	7	-3.737	-4.72	-1.100e-05	0.006	1.849	2.544
hon_000_22487	HFe ₂ Li ₂ Si	6	-4.392	-4.917	-3.000e-06	0.00605	0.878	2.774
hon_000_22498	Co ₄ Tm ₂	6	-6.018	-6.332	-7.000e-06	0.00368	0.545	0.537
hon_000_22516	Lu ₂ Ni ₃ Si	6	-5.587	-5.734	-5.000e-06	0.00631	0.453	0.378
hon_000_22539	Dy ₂ MgNa ₃	6	-2.099	-2.177	2.000e-06	0.00665	0.42	2.406
hon_000_22547	Br ₄ Gd ₂ Zr ₂	8	-4.281	-4.852	-3.000e-06	0.00524	1.565	1.127
hon_000_22552	CdEuNaSrYb ₂	6	-1.303	-1.447	1.000e-06	0.00498	0.647	0.5
hon_000_22573	Co ₂ Na ₂ SnZn	6	-2.939	-3.336	-1.600e-05	0.00555	1.519	2.09
hon_000_22597	FeNi ₄ Si	6	-5.997	-6.105	-2.000e-06	0.00576	0.572	0.379
hon_000_22605	Pt ₂ S ₄ Tb ₂	8	-4.878	-6.003	-2.000e-06	0.00515	2.054	4.068
hon_000_22658	Ag ₄ Dy ₂	6	-3.212	-3.616	-2.000e-06	0.00469	1.069	0.976
hon_000_22677	Ca ₂ GaSnTb ₂	6	-3.227	-3.674	-2.000e-06	0.00615	1.185	1.406
hon_000_22719	AsCr ₂ Mn ₂ Ni	6	-7.766	-7.807	-1.000e-06	0.00932	0.17	1.639
hon_000_22731	GdNd ₂ SnSr	5	-3.662	-4.078	-4.400e-05	0.00711	1.523	1.927
hon_000_22739	CdScSnTb ₂	5	-3.758	-4.395	2.000e-06	0.002	1.299	2.133
hon_000_22761	Co ₂ Sb ₂ Se	5	-4.762	-5.073	-1.300e-05	0.00811	0.584	1.53
hon_000_22764	Ca ₂ Ru ₂ Tl ₂	6	-3.682	-4.368	0.000e+00	0.00447	0.752	2.239
hon_000_22797	Cl ₄ Cu ₂ Gd ₂	8	-3.431	-4.123	0.000e+00	0.00577	1.522	1.454
hon_000_22800	GdMgNa ₂ Yb ₂	6	-1.684	-1.761	-1.100e-05	0.00264	1.035	1.618
hon_000_22804	CaDy ₂ LaSmTl	6	-3.744	-3.828	-8.000e-06	0.00508	0.399	2.478
hon_000_22811	Fe ₂ SiSn ₂	5	-5.172	-5.745	-4.000e-06	0.00361	0.777	1.525
hon_000_22864	Nd ₂ Pt ₂ S ₃ Tl	8	-4.777	-5.539	-4.000e-06	0.00378	1.364	3.556
hon_000_22925	CuRu ₂ Zn ₃	6	-3.932	-4.134	-1.000e-06	0.00685	0.316	1.003
hon_000_22987	Mn ₂ Tl ₃	5	-3.621	-4.44	8.000e-06	0.00804	1.922	1.623
hon_000_22990	BiDy ₃ GdTb	6	-4.63	-4.636	-1.000e-06	0.00298	0.288	0.239
hon_000_23034	AuCuGaMn ₂ Ti	6	-5.769	-5.962	-3.000e-06	0.00559	0.734	0.591
hon_000_23046	AlCo ₂ CuHoYb	6	-4.597	-4.691	4.000e-06	0.0072	0.546	1.844
hon_000_23047	Ge ₅ PrRu ₂	8	-5.733	-5.802	1.000e-06	0.006	0.349	0.334
hon_000_23049	Dy ₃ GaLiMg	6	-3.234	-3.441	-2.000e-06	0.00797	1.347	2.432

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_23125	AgNiSn ₂ Tb ₃	7	-4.405	-4.573	-1.000e-06	0.00671	0.523	0.428
hon_000_23178	H ₃ Co ₂ Na	6	-2.958	-3.955	-3.000e-06	0.00719	0.846	3.045
hon_000_23182	Co ₃ SiZr ₄	8	-7.587	-7.823	0.000e+00	0.00738	1.19	1.718
hon_000_23201	ISn ₂ Tb ₂ Tl	6	-3.554	-3.884	-2.000e-06	0.00589	0.887	1.267
hon_000_23207	CuNi ₂ Sc ₂ Sn	6	-5.446	-5.508	0.000e+00	0.00626	0.258	1.727
hon_000_23212	AlCo ₃ Tm ₂	6	-5.681	-5.843	3.000e-06	0.00693	0.516	1.185
hon_000_23213	CoFe ₂ PtU ₂	6	22.561	-8.82	-1.100e-05	0.00721	0.94	1.334
hon_000_23219	AuCo ₂ Nd ₂ Pd	6	-5.184	-5.559	-9.000e-06	0.00878	0.639	1.324
hon_000_23220	Cs ₂ SbSnYb ₂	6	-1.543	-2.448	-1.000e-06	0.00606	2.5	4.332
hon_000_23222	Cl ₃ IrYb ₂	6	-3.274	-4.356	-9.000e-06	0.00421	1.435	3.357
hon_000_23248	Ni ₂ PdSbSc	5	-5.491	-5.712	9.000e-06	0.00851	0.273	1.179
hon_000_23277	Gd ₂ Hg ₂ Tl ₄	8	-2.202	-2.565	0.000e+00	0.0031	0.854	0.692
hon_000_23310	Li ₂ Mn ₂ PS ₃	8	-5.695	-5.863	0.000e+00	0.00685	0.399	2.118
hon_000_23315	Al ₂ OsRu ₂ Si	6	-7.204	-7.451	-1.000e-06	0.00572	0.405	1.949
hon_000_23316	FeMnNi ₃ Sn	6	-5.89	-6.115	-2.400e-05	0.00873	0.397	0.422
hon_000_23319	DyGd ₂ Sn ₂ Te	6	-4.32	-4.947	-1.000e-06	0.00658	1.68	1.949
hon_000_23332	Dy ₂ La ₃ Sn	6	-4.753	-4.785	-2.000e-06	0.00323	0.14	1.122
hon_000_23355	BiCs ₄ Yb ₂	7	-1.47	-1.515	-1.000e-06	0.00319	0.659	1.67
hon_000_23367	AlGaNi ₂ Y	5	-4.848	-5.306	-3.400e-05	0.0058	1.271	2.122
hon_000_23412	Br ₄ Ni ₂	6	-2.159	-3.149	-2.000e-06	0.00954	1.025	0.742
hon_000_23421	Cs ₄ Dy ₂	6	-1.257	-1.705	-3.000e-06	0.00381	3.0	3.547
hon_000_23456	Co ₂ Ga ₂ TmYb	6	-4.316	-4.544	-4.000e-06	0.00759	0.668	1.322
hon_000_23481	AgFe ₂ ScSn ₃	7	-5.009	-5.184	0.000e+00	0.00956	1.345	1.668
hon_000_23491	Co ₂ GeNa ₄	7	-2.603	-2.909	-1.500e-05	0.00765	1.33	2.455
hon_000_23496	BiErInNd ₂ Sb	6	-4.397	-4.573	-2.000e-06	0.00664	0.677	0.724
hon_000_23503	Gd ₂ MgRu ₂ Sb ₂	7	-4.93	-5.646	2.000e-06	0.00682	0.751	1.522
hon_000_23539	Co ₃ CrGaGe	6	-6.177	-6.32	-2.000e-06	0.0068	0.389	0.396
hon_000_23547	Cd ₄ Ru ₂	6	-2.953	-3.281	3.000e-06	0.00827	0.535	1.269
hon_000_23548	Co ₃ Si ₃	6	-6.492	-6.514	1.000e-06	0.00735	0.065	0.792
hon_000_23550	AlCa ₂ Co ₂ Si	6	-4.364	-4.521	-9.000e-06	0.00697	0.478	1.032
hon_000_23589	Co ₂ Ga ₄	6	-3.946	-4.294	-4.000e-06	0.00559	0.717	1.058
hon_000_23590	AgGaLa ₂ Ru ₂	6	-5.469	-5.844	2.000e-06	0.0065	0.589	1.26
hon_000_23601	Na ₂ SnYb ₃	6	-1.808	-1.932	-3.000e-06	0.00297	0.409	0.507
hon_000_23612	Nd ₂ Sn ₃	5	-4.255	-4.754	-1.110e-04	0.00977	1.488	1.165
hon_000_23615	LuSn ₃ Tb ₂	6	-4.336	-4.638	-6.000e-06	0.00654	0.428	0.471
hon_000_23617	Al ₃ NdNi ₂ Pt	7	-4.955	-5.264	1.000e-06	0.00796	0.6	1.812
hon_000_23641	Cs ₄ Nd ₂	6	-1.516	-1.526	2.900e-06	0.00441	0.161	1.26
hon_000_23660	Co ₂ Ge ₂ Nd ₂	6	-4.716	-5.99	-1.000e-06	0.00793	0.766	0.87
hon_000_23671	CSnSr ₃ Tb ₂	7	-3.618	-3.914	0.000e+00	0.00913	1.033	0.729
hon_000_23672	Ag ₂ Pb ₂ Tb ₂	6	-3.564	-3.751	-2.000e-06	0.00523	0.63	0.435
hon_000_23680	Cs ₂ Gd ₂ KSb	6	-2.224	-2.619	1.000e-06	0.0084	1.875	4.07
hon_000_23686	Co ₂ SiTh ₂ Zn	6	-6.159	-6.331	-9.000e-06	0.00667	0.483	1.129
hon_000_23693	PdRu ₃ Zr ₂	6	-8.169	-8.493	1.000e-06	0.00506	0.283	0.199
hon_000_23709	CrNi ₂ Si ₃	6	-6.181	-6.458	-6.000e-06	0.00598	0.403	1.065
hon_000_23725	Co ₄ Dy ₃	7	-5.874	-5.983	-1.000e-06	0.0036	0.279	0.215
hon_000_23742	Ga ₃ Mn ₂ Na	6	-4.088	-4.575	-1.000e-06	0.00273	1.04	0.841
hon_000_23754	Fe ₂ PdSn ₃	6	-4.604	-5.292	0.000e+00	0.00434	0.665	0.715
hon_000_23780	PRu ₂ Sn ₂ Tm	6	-5.892	-6.261	-6.000e-06	0.00937	0.788	0.663
hon_000_23794	Fe ₂ Na ₄ NiTl	8	-2.938	-3.072	-4.000e-06	0.00755	1.019	2.429
hon_000_23815	AlFe ₃ Tm ₂	6	-5.991	-6.185	2.000e-06	0.00589	0.633	1.282
hon_000_23834	CCd ₄ SnTb ₂	8	-2.831	-3.14	0.000e+00	0.00477	0.703	1.537
hon_000_23861	Au ₂ GeNi ₃	6	-4.49	-4.529	0.000e+00	0.00779	0.196	0.214

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_23868	Co ₂ SbZr ₂	5	-7.065	-7.408	1.000e-06	0.00921	0.577	1.425
hon_000_23889	Sr ₂ Tb ₂ Tl ₂	6	-2.715	-2.967	-1.400e-05	0.00467	1.395	2.323
hon_000_23930	Ga ₂ Gd ₂ LaY	6	-4.45	-4.722	-1.600e-05	0.00877	0.587	1.846
hon_000_23940	MgNa ₂ Yb ₃	6	-1.256	-1.343	1.800e-06	0.00439	1.176	1.769
hon_000_23945	Cs ₃ Yb ₂	5	-0.806	-0.853	-1.000e-06	0.00169	0.642	0.775
hon_000_23954	Co ₃ Ga ₂ Mo	6	-6.256	-6.328	-9.000e-06	0.00629	0.131	0.783
hon_000_23959	Fe ₂ Ga ₂ Ru ₂	6	-6.6	-6.821	-9.000e-06	0.00562	0.923	1.527
hon_000_23979	Cd ₂ CoDy ₂ K ₂	7	-2.447	-2.639	-1.100e-05	0.00704	1.265	1.207
hon_000_23985	NaSbSnSrTb ₂	6	-3.197	-3.723	-1.000e-06	0.00587	1.065	1.97
hon_000_23992	CaNd ₂ Sn ₃	6	-4.033	-4.456	-1.100e-05	0.00673	1.766	1.554
hon_000_23997	PtRu ₂ SnU ₂	6	-8.469	-8.655	4.000e-06	0.00298	0.377	0.362
hon_000_24015	Ga ₃ Na ₂ Yb ₂	7	-2.042	-2.227	-4.000e-06	0.00372	1.249	2.746
hon_000_24020	Fe ₃ Mg ₃ Pt ₂	8	-4.938	-5.069	-4.000e-06	0.00429	0.464	1.386
hon_000_24022	Fe ₂ Sn ₂ Tm	5	-5.299	-5.795	0.000e+00	0.00685	1.306	2.853
hon_000_24053	Dy ₃ Nd ₂ Tl	6	-4.23	-4.289	7.000e-06	0.00276	0.369	0.279
hon_000_24089	GaMg ₂ NdTb ₂	6	-3.236	-3.488	-4.000e-06	0.00643	1.082	1.974
hon_000_24103	Al ₂ Ru ₂ TiU	6	-7.331	-7.644	-1.000e-06	0.00579	0.608	0.587
hon_000_24104	Ga ₃ Mn ₂ Mo	6	-5.784	-6.102	1.000e-06	0.00701	0.246	1.855
hon_000_24114	Dy ₃ GaGeSe ₃	8	-4.201	-5.227	1.000e-06	0.00867	1.112	2.332
hon_000_24140	CdGd ₄ Sn	6	-3.863	-4.132	-5.000e-06	0.00362	1.62	2.986
hon_000_24167	AlPt ₂ Ru ₂	5	-6.398	-6.895	-1.000e-06	0.00384	0.473	1.241
hon_000_24217	La ₂ SnTb ₃	6	-4.548	-4.711	0.000e+00	0.0048	0.469	0.264
hon_000_24233	Br ₄ Ir ₂ Nd ₂	8	-4.328	-4.998	-1.300e-05	0.00619	1.729	2.434
hon_000_24265	Co ₃ GaMn ₂	6	-6.688	-6.918	-7.000e-06	0.00812	0.389	0.281
hon_000_24274	LiMn ₃ Si ₂	6	-6.568	-6.724	-5.000e-06	0.00817	0.457	1.064
hon_000_24277	Al ₂ Ru ₂ Tb	5	-5.736	-6.372	-1.000e-06	0.00294	0.594	2.176
hon_000_24322	Cl ₄ Dy ₂ Pt ₂	8	-3.911	-4.84	-4.000e-06	0.00707	0.861	1.937
hon_000_24337	Rh ₂ Sn ₄ Yb ₂	8	-4.362	-4.634	-2.000e-06	0.00767	0.995	1.751
hon_000_24348	AlCo ₃ Mn ₂	6	-6.917	-7.135	-3.000e-06	0.00812	0.584	0.312
hon_000_24358	Al ₃ CoNi ₂	6	-5.051	-5.293	-9.000e-06	0.00386	0.256	0.866
hon_000_24375	Fe ₂ Mn ₂ SiV	6	-8.24	-8.299	-1.000e-06	0.00765	0.123	0.123
hon_000_24394	Ga ₂ Pr ₂ Ru ₂	6	-5.418	-5.933	-3.000e-06	0.00438	1.054	1.033
hon_000_24416	AlCo ₄ Ti	6	-6.651	-6.844	3.000e-06	0.00316	0.884	0.799
hon_000_24418	CaCdDy ₄	6	-3.31	-3.506	0.000e+00	0.00181	1.403	1.437
hon_000_24445	GaMn ₂ Zn ₃	6	-3.75	-3.887	-1.000e-06	0.00539	0.339	0.204
hon_000_24479	Co ₂ Pt ₂ Sn	5	-5.698	-6.023	1.000e-06	0.004	0.725	1.467
hon_000_24487	Dy ₅ In	6	-4.354	-4.321	-8.000e-06	0.00417	0.5	1.264
hon_000_24489	Gd ₅ U	6	-5.295	-5.359	-4.000e-05	0.00321	0.223	0.231
hon_000_24490	Cs ₃ Nd ₂ Tl	6	-1.855	-2.043	-1.000e-06	0.00583	1.469	3.912
hon_000_24498	Cd ₂ Gd ₂ Sn ₂	6	-3.158	-3.508	0.000e+00	0.00442	1.47	2.019
hon_000_24557	Fe ₂ Pt ₂ SiSn	6	-5.881	-6.321	-3.000e-06	0.00672	1.194	1.866
hon_000_24590	AgLa ₂ Ru ₂ SbTe	7	-5.325	-5.748	-1.000e-06	0.00697	0.545	1.303
hon_000_24623	Au ₂ Dy ₃ In	6	-4.56	-4.334	-1.000e-06	0.00401	0.336	0.259
hon_000_24638	Al ₃ Fe ₂ GaY ₂	8	-5.324	-5.48	-5.000e-06	0.00581	0.686	0.631
hon_000_24644	Co ₂ Ga ₂ Li	5	-4.118	-4.303	0.000e+00	0.00931	0.385	2.075
hon_000_24649	Co ₂ GaGe ₂ MnNa	7	-4.775	-4.976	0.000e+00	0.00445	0.207	0.948
hon_000_24658	AlGaOsRu ₂ Si	6	-6.943	-7.197	1.000e-06	0.00432	0.46	1.12
hon_000_24678	Al ₄ Co ₂ Dy	7	-4.79	-4.989	-1.200e-05	0.00567	1.056	1.971
hon_000_24688	Fe ₂ GaMg ₂ Pt ₂ Zn	8	-4.381	-4.62	-7.000e-06	0.00771	0.647	2.321
hon_000_24702	PPtRu ₂ SbZr ₂	7	-7.516	-7.941	-3.000e-06	0.00207	0.937	0.515
hon_000_24705	AlPt ₃ Ru ₂	6	-6.694	-7.038	1.000e-06	0.00272	0.642	1.891
hon_000_24710	Gd ₃ SnYb ₂	6	-3.373	-3.609	0.000e+00	0.00641	0.954	0.8

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_24784	AlPt ₃ Ru ₂	6	-6.641	-7.028	-7.000e-06	0.00438	0.551	0.386
hon_000_24823	Nd ₂ Rh ₂ Se ₄	8	-5.019	-5.79	0.000e+00	0.00444	1.199	3.206
hon_000_24862	ClNaSeSnYb ₂	6	-2.702	-3.472	-1.400e-05	0.00375	1.751	3.085
hon_000_24878	Cl ₅ FeTb ₂	8	-4.415	-4.661	-7.000e-06	0.00593	0.527	0.531
hon_000_24899	Ga ₃ Tb ₃	6	-3.711	-4.221	-1.000e-06	0.00801	1.458	1.207
hon_000_24917	AlGd ₂ MgSr ₂	6	-2.745	-2.887	-1.000e-06	0.00349	0.919	1.623
hon_000_24948	Ca ₂ Co ₂ CuPt	6	-4.581	-4.662	-1.000e-06	0.005	0.39	0.357
hon_000_24955	GaRh ₂ SrTe ₂ Yb ₂	8	-3.989	-4.353	-3.000e-06	0.00491	0.876	1.376
hon_000_24959	DySn ₂ Tb ₃	6	-4.368	-4.668	-3.100e-05	0.00672	0.596	0.385
hon_000_24976	AuRu ₂ Zn ₄	7	-3.422	-3.62	0.000e+00	0.00522	0.298	0.936
hon_000_24988	RbSbSnYb ₂	5	-2.067	-2.89	-1.000e-06	0.00457	1.594	3.921
hon_000_25027	Dy ₄ GdSn	6	-4.59	-4.644	-7.000e-06	0.00381	0.396	0.484
hon_000_25031	Cl ₄ Mn ₂ Nd ₂	8	-4.403	-5.122	-1.000e-06	0.00559	1.715	2.097
hon_000_25062	Ru ₂ Zr ₄	6	-8.704	-8.912	-7.000e-06	0.00603	0.686	0.679
hon_000_25068	CoGe ₂ Ni ₂	5	-5.185	-5.48	1.000e-06	0.00832	0.526	1.256
hon_000_25079	Cl ₆ Tb ₂	8	-4.791	-4.816	-1.000e-06	0.00597	0.219	0.293
hon_000_25092	Cl ₄ PtTb ₂	7	-3.836	-4.588	-1.000e-06	0.00284	1.431	1.688
hon_000_25098	AlAuCe ₂ Fe ₂ Li	7	-5.197	-5.461	-6.000e-06	0.0097	0.881	1.51
hon_000_25134	BaCs ₂ SbYb ₂	6	-1.787	-1.83	-1.000e-05	0.00305	0.425	0.472
hon_000_25139	AlCaFe ₂ Pd	5	-4.729	-5.458	-3.000e-06	0.00369	0.818	0.76
hon_000_25200	AuFe ₃ ZnZr	6	-5.743	-6.077	4.000e-06	0.00673	0.61	1.322
hon_000_25203	Gd ₂ Rb ₄	6	-1.278	-1.59	1.190e-05	0.00479	2.679	3.827
hon_000_25246	BaCsInSrYb ₂	6	-1.646	-1.6	9.000e-07	0.00285	1.416	2.947
hon_000_25250	Ge ₂ Ru ₂ U ₂	6	-8.189	-8.527	0.000e+00	0.00594	0.418	1.558
hon_000_25254	Cl ₆ Tb ₂	8	-4.744	-4.815	-2.000e-06	0.00682	0.33	0.304
hon_000_25266	Co ₃ CuTm ₂	6	-5.594	-5.762	-2.000e-06	0.00417	0.523	0.499
hon_000_25270	Sn ₃ Yb ₂ Zr	6	-3.788	-4.243	0.000e+00	0.00968	0.633	0.347
hon_000_25298	KNa ₂ Ru ₂	5	-3.589	-3.865	-3.000e-06	0.00631	1.172	2.011
hon_000_25304	Br ₄ Pt ₂ Yb ₂	8	-3.225	-3.752	-2.000e-06	0.00471	1.531	2.161
hon_000_25325	Ag ₃ SbYb ₃	7	-2.304	-2.843	-1.000e-06	0.00759	1.224	3.283
hon_000_25382	Cl ₄ NbTb ₂	7	-4.163	-4.957	-1.700e-05	0.00453	1.206	5.084
hon_000_25395	AlCuNi ₂ Y ₂	6	-5.499	-5.582	5.000e-06	0.00471	0.403	1.725
hon_000_25397	Gd ₂ LuMg ₂ U	6	-4.158	-4.272	0.000e+00	0.00618	0.335	0.318
hon_000_25401	Ga ₃ Nd ₂ Sn	6	-3.584	-3.951	4.000e-06	0.00924	0.709	1.395
hon_000_25415	Fe ₂ Pd ₃ U	6	-6.766	-7.312	-4.000e-06	0.00913	0.459	0.662
hon_000_25430	CrGe ₂ Ni ₂ Si	6	-5.289	-5.882	0.000e+00	0.00687	0.41	0.599
hon_000_25444	Gd ₂ Ru ₂ Sb ₂	6	-5.322	-6.468	0.000e+00	0.00834	1.517	1.148
hon_000_25466	Gd ₄ LuSb	6	-4.627	-4.748	-1.000e-06	0.00854	0.447	1.231
hon_000_25494	Cl ₄ Ir ₂ Tb ₂	8	-4.553	-5.157	-4.000e-06	0.00781	1.391	1.523
hon_000_25511	Cd ₄ Fe ₂ Pd ₂	8	-3.325	-3.584	-2.100e-05	0.00687	1.19	0.903
hon_000_25535	AuFe ₂ Li ₂ MgNaSi	8	-3.538	-3.859	-2.000e-06	0.00695	0.893	2.171
hon_000_25547	Ba ₃ SrYb ₂	6	-1.505	-1.665	-5.700e-06	0.00121	1.263	2.258
hon_000_25558	Co ₃ GeLiU	6	-6.392	-6.541	-1.200e-05	0.00297	0.235	0.853
hon_000_25576	SnTb ₂ Tl ₃	6	-3.133	-3.52	-3.000e-06	0.00238	0.717	0.71
hon_000_25584	Dy ₂ Eu ₂ Ga ₂ Ru ₂	8	-4.707	-4.932	-2.000e-06	0.00486	0.482	1.257
hon_000_25595	Ga ₅ NaYb ₂	8	-2.371	-2.652	-1.000e-06	0.0073	0.974	1.466
hon_000_25629	Fe ₂ Mg ₂ PtSn	6	-4.48	-4.813	-4.000e-06	0.00633	1.142	0.61
hon_000_25631	Fe ₂ GeTbZn	5	-4.83	-5.155	-1.000e-06	0.00663	0.738	1.41
hon_000_25673	Cd ₂ Ru ₂ Sn	5	-4.259	-4.401	-4.000e-06	0.00407	0.247	0.286
hon_000_25674	Au ₂ Fe ₂ Sb	5	-4.85	-5.026	-1.300e-05	0.00558	0.307	1.098
hon_000_25687	Br ₄ Pd ₂ Tb ₂	8	-3.697	-4.361	0.000e+00	0.0057	1.386	2.147
hon_000_25693	Mn ₂ Y ₃	5	-6.3	-7.093	-1.000e-06	0.00996	0.852	0.791

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_25704	AlFe ₃ Si ₂	6	-6.6	-6.778	2.000e-05	0.00608	0.522	0.503
hon_000_25773	CsRb ₂ Yb ₂	5	-0.73	-0.866	-9.000e-07	0.00323	0.969	4.677
hon_000_25823	Br ₄ PtTb ₂	7	-3.383	-4.499	-2.000e-06	0.00863	1.67	2.494
hon_000_25832	Gd ₃ MgSn ₂	6	-3.916	-4.343	-1.500e-05	0.004	1.939	1.823
hon_000_25857	Ni ₂ PtSi ₃	6	-5.677	-5.868	-4.500e-05	0.00532	0.33	1.787
hon_000_25877	Gd ₂ Ge ₂ Sr ₃	7	-3.229	-3.576	-1.000e-06	0.00431	1.3	1.729
hon_000_25946	Pd ₂ Ru ₂ Sb	5	-6.251	-6.435	6.000e-06	0.00652	0.489	1.219
hon_000_25950	Li ₂ Mg ₂ Nd ₂	6	-2.52	-2.635	-2.000e-06	0.00362	0.621	0.472
hon_000_25989	Al ₂ Ni ₄	6	-4.988	-5.333	-1.900e-05	0.0071	0.977	1.666
hon_000_25996	BaNd ₂ Tl ₃	6	-2.964	-3.233	0.000e+00	0.00381	1.105	0.771
hon_000_25999	Bi ₂ Dy ₂ Tl ₂	6	-3.487	-3.886	-4.100e-05	0.00982	1.23	2.433
hon_000_26027	Nd ₂ Sb ₂ Sn ₃	7	-4.331	-4.658	1.000e-06	0.00684	0.842	1.561
hon_000_26031	Br ₄ Gd ₂ Pd	7	-3.558	-4.315	-1.000e-06	0.00568	2.485	2.41
hon_000_26044	Dy ₂ GaNa ₂ Si ₂	7	-3.539	-3.72	-1.000e-06	0.00804	1.114	2.452
hon_000_26083	Pr ₂ Ru ₂ Sb	5	-5.758	-6.773	4.000e-06	0.00633	1.104	1.02
hon_000_26104	Cl ₄ RuYb ₂	7	-3.277	-4.28	-2.000e-06	0.00609	1.789	2.522
hon_000_26113	Gd ₂ Sn ₄	6	-4.154	-4.641	-3.000e-06	0.00949	1.609	2.161
hon_000_26131	AuFe ₃ Gd ₂	6	-5.926	-6.115	-2.200e-05	0.00539	0.505	1.055
hon_000_26138	Cd ₃ SbSnTb ₂	7	-2.801	-3.146	-7.000e-06	0.00759	1.417	3.308
hon_000_26226	Al ₃ Ni ₃	6	-4.896	-4.979	4.000e-06	0.00601	0.253	0.921
hon_000_26265	Co ₃ SbTb	5	-5.77	-6.097	-2.000e-05	0.00685	0.57	1.191
hon_000_26271	Fe ₂ Se ₄	6	-3.841	-5.151	-1.000e-06	0.00479	1.183	0.955
hon_000_26273	Bi ₃ Yb ₃	6	-3.102	-3.434	1.000e-06	0.00164	1.261	1.077
hon_000_26295	AlCdDy ₄	6	-3.679	-3.992	0.000e+00	0.00419	1.411	2.247
hon_000_26319	Co ₂ Dy ₄	6	-5.328	-5.485	-1.300e-05	0.00692	0.429	0.219
hon_000_26332	Cl ₄ Gd ₂ Ir	7	-4.096	-4.985	-5.000e-06	0.00702	1.419	1.333
hon_000_26350	Cl ₄ Tb ₂ Zr ₂	8	-4.633	-5.191	0.000e+00	0.00541	0.869	2.203
hon_000_26376	Ga ₂ LiNi ₂ Sn	6	-3.649	-3.938	-1.600e-05	0.00722	0.593	0.73
hon_000_26388	BiCa ₂ Ru ₂	5	-4.879	-5.335	1.000e-06	0.00321	1.112	1.578
hon_000_26389	Cs ₃ RbYb ₂	6	-0.8	-0.883	-1.300e-06	0.00245	2.268	6.001
hon_000_26411	CuLaLiNi ₂ P	6	-4.758	-4.953	-4.000e-06	0.00592	0.473	3.621
hon_000_26413	Cl ₄ Gd ₂ Ir ₂	8	-4.397	-5.295	-9.000e-06	0.00486	1.816	3.97
hon_000_26426	Nd ₂ Sn ₄	6	-4.362	-4.547	1.000e-06	0.00675	0.365	2.287
hon_000_26427	CuNd ₂ Ru ₂ Zn	6	-5.247	-5.606	1.000e-06	0.00739	0.556	1.281
hon_000_26479	GaMn ₄ Ni	6	-7.122	-7.305	1.000e-06	0.00721	0.152	0.941
hon_000_26502	Al ₃ PdRu ₂	6	-5.848	-6.104	0.000e+00	0.00854	0.502	1.054
hon_000_26506	Co ₄ Ga ₂	6	-5.565	-5.675	-2.000e-06	0.00421	0.227	1.568
hon_000_26528	ErGaNi ₄	6	-5.059	-5.245	-8.500e-05	0.00963	0.295	0.257
hon_000_26573	Fe ₄ Pt ₂	6	-7.253	-7.354	1.000e-06	0.00515	0.178	0.865
hon_000_26581	AlNi ₂ PdTh	5	-5.676	-6.005	-6.000e-06	0.00696	0.582	1.76
hon_000_26611	Cl ₄ Gd ₂ Ir ₂	8	-4.455	-5.251	-1.000e-05	0.00757	1.568	2.213
hon_000_26619	CeSnTb ₂ Tl ₂	6	-3.709	-4.155	-1.500e-05	0.00756	1.209	2.655
hon_000_26668	Dy ₃ MgTb ₂	6	-3.997	-4.006	2.000e-06	0.00142	0.134	1.105
hon_000_26680	Sn ₃ Tb ₂ Zr	6	-5.03	-5.251	-6.000e-06	0.00462	0.569	1.277
hon_000_26681	Cs ₃ Nd ₂	5	-1.72	-1.751	-9.950e-05	0.00351	0.89	2.609
hon_000_26685	Fe ₂ InPt ₂	5	-5.913	-6.136	7.000e-06	0.00658	0.564	1.852
hon_000_26695	Al ₂ Cu ₂ Ru ₂	6	-5.466	-5.746	-8.300e-05	0.00847	0.437	1.053
hon_000_26750	Au ₂ EuRu ₂	5	-4.623	-5.422	-8.000e-06	0.00513	0.676	0.422
hon_000_26751	GeSe ₃ SiTb ₂ Tl	8	-3.969	-4.599	-3.000e-05	0.00732	1.804	2.062
hon_000_26760	Al ₂ Ru ₂ SbTb ₂	7	-5.399	-6.057	-4.000e-06	0.00498	0.853	1.591
hon_000_26767	Nd ₂ Tl ₄	6	-2.957	-3.325	-1.000e-06	0.00453	1.19	1.966
hon_000_26772	Nd ₂ PPdSe ₃	7	-4.818	-5.599	-1.000e-06	0.00569	1.807	2.636

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_26786	BaCa ₃ Gd ₂	6	-2.65	-2.66	1.000e-06	0.00193	0.189	0.146
hon_000_26813	Ce ₄ Nd ₂	6	-5.148	-5.416	5.000e-06	0.00887	0.611	0.494
hon_000_26823	AgRu ₂ Sm ₂ Sn	6	-5.628	-5.914	0.000e+00	0.00715	0.72	1.365
hon_000_26837	Dy ₂ Th ₂ Zr ₂	6	-6.66	-6.739	0.000e+00	0.00392	0.333	0.254
hon_000_26869	Nd ₂ Pt ₂ Se ₃	7	-4.859	-5.666	0.000e+00	0.0042	1.651	2.324
hon_000_26925	AcCaCdYb ₃	6	-1.806	-1.911	0.000e+00	0.00314	0.906	1.03
hon_000_26985	Co ₂ CrGaGeSi	6	-5.929	-6.088	-3.000e-06	0.00797	0.886	2.089
hon_000_26996	Ag ₂ Al ₂ Dy ₃ Pd	8	-4.056	-4.365	-6.000e-06	0.00283	2.206	2.202
hon_000_27000	Cl ₄ Gd ₂ Pd ₂	8	-3.904	-4.818	-2.000e-06	0.00486	1.869	1.91
hon_000_27009	Cd ₂ Dy ₂ NiPdSr ₂	8	-3.05	-3.257	-1.000e-06	0.00834	0.578	2.83
hon_000_27016	Ni ₂ PtSi ₃	6	-5.631	-5.816	-3.500e-05	0.00535	0.292	0.227
hon_000_27039	Co ₂ Ga ₂ Gd ₂ Ge	7	-4.762	-5.051	-4.000e-06	0.00587	0.889	1.97
hon_000_27042	Br ₂ ClGa ₂ Gd ₂ S	8	-3.242	-4.106	0.000e+00	0.00898	1.769	3.374
hon_000_27053	Al ₃ Co ₂ Ga	6	-4.708	-4.916	-1.400e-05	0.00932	1.194	1.527
hon_000_27108	Ca ₂ Ru ₂ Te	5	-4.16	-5.484	-3.000e-06	0.00969	1.598	0.994
hon_000_27131	Ag ₂ LaRu ₂ SnY	7	-5.561	-5.706	-1.000e-06	0.00654	0.502	0.589
hon_000_27158	Br ₂ LaNd ₂ Rh ₂ Se	8	-4.85	-5.467	0.000e+00	0.00645	1.174	1.848
hon_000_27192	Ce ₂ GaRu ₂ Tl	6	-5.933	-6.088	-3.000e-06	0.00499	0.951	0.81
hon_000_27199	BaSbTb ₂ Tl	5	-3.245	-3.966	-2.000e-06	0.00566	1.534	3.68
hon_000_27208	Cs ₃ Nd ₂ Rb	6	-1.533	-1.615	-1.460e-05	0.00173	0.91	4.887
hon_000_27214	AsFe ₃ Si	5	-6.589	-6.798	-2.500e-05	0.00511	0.274	0.31
hon_000_27220	Al ₂ Br ₄ Tb ₂	8	-3.028	-3.798	-5.000e-06	0.00698	1.602	2.734
hon_000_27242	HCaMgNpRu ₂	6	-5.28	-6.355	-1.100e-05	0.00521	1.173	1.827
hon_000_27260	Cl ₄ Pt ₂ Tb ₂	8	-4.116	-4.864	-2.000e-06	0.00544	2.323	3.489
hon_000_27262	Co ₄ Si ₂	6	-6.605	-6.8	-1.000e-06	0.00563	0.562	0.582
hon_000_27281	AgSn ₂ SrYb ₂	6	-2.452	-3.009	-2.000e-05	0.00528	1.309	1.1
hon_000_27312	Ce ₂ Co ₂ GaIn	6	-5.389	-5.419	-1.000e-06	0.00429	0.519	1.216
hon_000_27315	Br ₄ Ir ₂ Nd ₂	8	-4.305	-4.917	-1.200e-05	0.00756	1.366	2.249
hon_000_27318	CdNd ₂ Sr ₂	5	-2.357	-2.607	-4.000e-06	0.00251	0.857	1.961
hon_000_27333	Al ₂ MoRu ₂ Ta	6	-8.231	-8.3	-6.000e-06	0.0055	0.214	1.064
hon_000_27336	HgNaPbYb ₂	5	-1.568	-1.979	-1.100e-06	0.00538	1.935	2.432
hon_000_27348	BeCuGaNi ₂ Os	6	-5.335	-5.452	-3.000e-06	0.00639	0.688	1.248
hon_000_27373	Ga ₂ Tb ₂ Te ₃	7	-3.805	-4.216	0.000e+00	0.00715	0.892	0.618
hon_000_27397	Ga ₃ MgMn ₂	6	-4.419	-4.602	-1.000e-06	0.0045	0.576	1.917
hon_000_27417	CeGe ₂ Ni ₂	5	-5.144	-5.295	2.000e-06	0.00714	0.226	0.323
hon_000_27469	Co ₂ PtU ₃	6	21.437	-9.088	6.000e-06	0.00872	0.72	2.942
hon_000_27479	Na ₂ Sn ₂ Yb ₂	6	-2.253	-2.553	-2.000e-06	0.00386	1.03	0.943
hon_000_27494	Sn ₄ Yb ₂	6	-3.005	-3.559	-2.000e-06	0.00624	1.583	1.05
hon_000_27510	Al ₂ AuRu ₂ Tb	6	-5.209	-5.8	-5.000e-06	0.00662	0.615	1.311
hon_000_27513	Co ₂ LiNi ₂ PSn	7	-4.877	-5.398	-3.000e-06	0.00454	0.695	2.388
hon_000_27539	Ba ₂ InYb ₃	6	-2.019	-1.891	-5.000e-06	0.00329	1.435	2.106
hon_000_27553	Rh ₂ Sn ₃ Tb ₃	8	-5.285	-5.633	-5.000e-06	0.00521	0.912	2.523
hon_000_27575	Ru ₂ Zr ₄	6	-8.595	-8.892	-1.000e-06	0.00758	0.621	0.687
hon_000_27576	C ₂ GaTb ₄ Zn	8	-4.729	-5.142	0.000e+00	0.00616	0.733	2.286
hon_000_27597	Co ₂ SbTb ₂	5	-5.483	-5.909	-2.000e-05	0.00745	0.858	0.794
hon_000_27648	Ni ₄ Sn ₂ Y	7	-5.325	-5.426	-2.000e-06	0.00657	0.06	0.888
hon_000_27662	Al ₂ Nd ₂ Ni ₂	6	-4.923	-4.957	3.000e-06	0.00329	0.236	0.241
hon_000_27696	LuTb ₂ Tl ₂ Zr	6	-4.306	-4.582	-1.700e-05	0.00576	1.052	1.618
hon_000_27720	GaGd ₂ Mg ₂ Sc	6	-3.489	-3.744	0.000e+00	0.0049	0.305	1.712
hon_000_27751	Al ₂ GaNi ₂ Rh	6	-5.142	-5.269	-4.000e-06	0.00972	0.177	0.28
hon_000_27764	Cl ₄ Tb ₂ Ti	7	-4.112	-4.681	2.000e-06	0.00581	1.438	1.925
hon_000_27776	Co ₂ Lu ₂ Ni ₄	8	-5.688	-5.801	-4.000e-05	0.00996	0.266	1.41

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_27795	Co ₃ GeLi ₄	8	-3.889	-4.025	-1.000e-06	0.00617	0.429	1.401
hon_000_27805	Cd ₂ SnYb ₃	6	-1.743	-1.999	1.000e-06	0.00389	1.356	2.634
hon_000_27815	Gd ₂ MgTbZr ₂	6	-5.136	-5.243	4.000e-06	0.00244	0.431	1.196
hon_000_27832	GaMn ₂ PdV ₂	6	-7.166	-7.422	-2.000e-06	0.00252	0.641	1.962
hon_000_27841	Co ₃ GeSi	5	-6.099	-6.164	-2.000e-05	0.00837	0.234	1.87
hon_000_27843	Dy ₂ Sn ₂ Tb ₂	6	-4.374	-4.797	-1.000e-06	0.00314	0.785	1.48
hon_000_27865	Ga ₂ Ni ₃ Zn	6	-4.026	-4.121	-3.000e-06	0.00633	0.329	1.032
hon_000_27916	Co ₅ Ni	6	-6.424	-6.556	-6.000e-06	0.00597	0.247	0.121
hon_000_27919	CuPr ₃ Ru ₂ Zn	7	-5.076	-5.373	-2.000e-06	0.00433	1.51	1.669
hon_000_27958	Nd ₂ Se ₄ Ti ₂	8	-5.401	-6.121	-3.000e-06	0.00486	2.203	2.712
hon_000_27973	CoGa ₂ Sn ₂ Yb ₂	7	-3.288	-3.787	-8.000e-06	0.00598	1.908	2.619
hon_000_27980	Al ₂ Fe ₂ Li ₂	6	-4.544	-4.655	-2.000e-06	0.00454	0.419	0.376
hon_000_28007	Sn ₄ Tb ₂	6	-3.876	-4.487	1.000e-06	0.0026	0.756	0.73
hon_000_28037	Gd ₄ SnSr	6	-3.994	-4.11	0.000e+00	0.00411	0.264	1.334
hon_000_28047	IrSn ₃ Tb ₃	7	-5.11	-5.509	-3.000e-06	0.0044	0.708	2.455
hon_000_28050	GeLa ₂ Ru ₃	6	-6.9	-7.267	0.000e+00	0.00918	1.009	0.77
hon_000_28076	Dy ₂ Fe ₂ MgSi ₂	7	-5.328	-5.527	-1.300e-05	0.00849	0.624	1.829
hon_000_28107	Fe ₂ NdPt ₄	7	-6.393	-6.604	-2.000e-06	0.00627	0.623	1.06
hon_000_28116	AlEr ₂ PdRu ₂	6	-5.867	-6.49	-6.000e-06	0.00649	0.665	1.306
hon_000_28128	Sn ₂ Tb ₂ Th ₂	6	-5.313	-5.716	-2.000e-06	0.00288	0.604	1.62
hon_000_28136	CaCdIrSnSrTb ₂	7	-3.807	-4.033	-1.000e-06	0.00349	0.563	2.425
hon_000_28147	Eu ₂ In ₂ Tb ₂	6	-2.957	-3.314	0.000e+00	0.00716	1.487	2.72
hon_000_28170	Al ₂ Co ₄	6	-5.969	-6.119	2.000e-06	0.00846	0.299	0.888
hon_000_28192	Cs ₄ Nd ₂	6	-1.497	-1.611	0.000e+00	0.0045	2.307	4.433
hon_000_28201	Al ₄ Co ₂	6	-4.755	-5.257	-1.000e-06	0.00928	1.011	1.992
hon_000_28213	Co ₃ Si ₃	6	-6.16	-6.606	-3.000e-06	0.00975	0.453	2.376
hon_000_28239	AgGa ₃ Nd ₂ Tl	7	-3.341	-3.614	-2.000e-06	0.00982	1.025	2.644
hon_000_28249	CaRu ₂ SiZn ₂	6	-4.289	-4.765	0.000e+00	0.0068	1.441	3.566
hon_000_28258	Br ₄ PdTb ₂	7	-3.261	-4.431	-3.000e-06	0.00724	2.016	3.019
hon_000_28288	AgPrRu ₂ SbTh	6	-6.282	-6.584	1.000e-06	0.00403	0.593	2.012
hon_000_28310	AlGeNi ₃ Si	6	-5.2	-5.295	-9.000e-06	0.00489	0.287	0.934
hon_000_28326	Fe ₂ Ga ₃ Li	6	-4.35	-4.625	0.000e+00	0.00317	0.5	1.38
hon_000_28333	Na ₃ SrTb ₂	6	-2.121	-2.144	-1.000e-06	0.0071	0.365	3.251
hon_000_28357	Cl ₃ IND ₂ O ₈	7	-4.153	-5.125	0.000e+00	0.00798	2.196	2.305
hon_000_28382	Cl ₄ PdTb ₂	7	-3.567	-4.806	1.000e-06	0.00845	1.645	3.61
hon_000_28415	Al ₂ Ni ₂ V ₂	6	-6.087	-6.285	-3.900e-05	0.00855	0.351	0.303
hon_000_28422	BaSn ₄ TlYb ₂	8	-2.804	-3.175	-1.000e-06	0.00536	1.191	0.847
hon_000_28434	KNd ₂ Rh ₂ S ₃	8	-4.997	-5.599	0.000e+00	0.00634	1.172	1.057
hon_000_28447	Cd ₂ MgSrTb ₂	6	-2.242	-2.421	0.000e+00	0.00225	1.246	1.455
hon_000_28462	LiNi ₂ Sn	4	-3.859	-4.487	-1.000e-06	0.00595	1.075	2.796
hon_000_28472	Ge ₃ Nd ₃ Ru ₂	8	-5.785	-6.154	-6.000e-06	0.00588	0.718	1.026
hon_000_28503	HgRu ₂ SnTm ₂	6	-4.922	-5.449	-9.000e-06	0.00592	0.513	0.472
hon_000_28532	MgNd ₂ P ₄	7	-4.72	-5.569	0.000e+00	0.00261	1.669	2.553
hon_000_28535	Dy ₄ HoMg	6	-3.956	-3.991	2.000e-06	0.00451	0.272	0.199
hon_000_28600	CaLi ₂ MgTb ₂	6	-2.522	-2.566	-1.000e-06	0.002	0.277	0.315
hon_000_28625	LaTb ₄ Tl	6	-4.068	-4.265	0.000e+00	0.0042	0.492	0.374
hon_000_28682	Cl ₃ PdSYb ₂	7	-3.387	-4.25	-6.000e-06	0.00341	1.61	4.145
hon_000_28715	Al ₂ Ru ₂ Ti ₂	6	-7.202	-7.496	-1.000e-06	0.00165	1.368	1.214
hon_000_28725	Br ₃ PtYb ₂	6	-2.739	-3.621	-1.000e-06	0.00649	2.124	3.393
hon_000_28739	AlAsNi ₂ Ti	5	-5.585	-5.782	0.000e+00	0.00486	0.649	2.314
hon_000_28753	CeGa ₂ MoRu ₂	6	-6.633	-7.064	1.000e-06	0.00477	0.391	1.223
hon_000_28763	Gd ₃ LaSn ₂	6	-4.728	-4.87	-9.000e-06	0.00562	0.489	0.283

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_28768	Fe ₂ Ga ₃ V	6	-5.47	-5.615	1.000e-06	0.00491	0.775	1.886
hon_000_28789	InPb ₃ Yb ₂	6	-3.11	-3.028	2.000e-06	0.00374	0.427	0.39
hon_000_28813	Dy ₂ P ₂ S ₄	8	-4.462	-5.638	-1.000e-06	0.00922	1.68	1.764
hon_000_28839	Rb ₄ Tb ₂	6	-1.44	-1.641	-1.900e-06	0.00333	2.636	2.824
hon_000_28857	Cl ₃ IPdTb ₂	7	-3.442	-4.492	0.000e+00	0.00562	1.195	3.031
hon_000_28861	Na ₃ Tb ₃	6	-2.551	-2.688	6.000e-06	0.00368	0.644	0.458
hon_000_28867	GeNi ₂ Sn ₂ Zr ₂	7	-5.361	-5.866	-2.000e-06	0.00913	0.707	1.035
hon_000_28875	AgAlRu ₂ Tb ₂	6	-5.225	-5.876	-6.000e-06	0.00647	0.88	0.762
hon_000_28899	AlFe ₂ PdZr ₂	6	-6.853	-7.303	-2.000e-06	0.00416	1.029	2.309
hon_000_28901	Dy ₅ PdSb	7	-4.749	-5.004	0.000e+00	0.00206	0.591	0.651
hon_000_28904	Cd ₃ GaRu ₂	6	-3.292	-3.66	-2.000e-06	0.00429	0.678	0.505
hon_000_28952	Cd ₂ Gd ₂ SrYb	6	-2.22	-2.366	-6.000e-06	0.00519	1.989	3.317
hon_000_28974	Cd ₄ Yb ₂	6	-0.879	-1.288	0.000e+00	0.0026	1.644	1.782
hon_000_28981	AlSr ₂ Tb ₂ Tl	6	-2.859	-3.226	-1.000e-06	0.00481	0.605	1.5
hon_000_28982	Ca ₂ Co ₂ SiZn	6	-3.917	-4.11	-1.000e-06	0.00725	0.581	1.271
hon_000_29005	GaPt ₂ Ru ₂	5	-6.362	-6.59	-4.000e-06	0.00742	0.38	1.313
hon_000_29023	As ₃ Cu ₂ GaNi ₂	8	-4.296	-4.423	-3.000e-06	0.00837	0.461	1.678
hon_000_29032	CdGaPr ₂ Ru ₂	6	-5.271	-5.42	4.000e-06	0.00581	0.636	1.338
hon_000_29058	Fe ₂ Gd ₂ Zn ₂	6	-4.515	-4.706	-3.000e-06	0.00637	0.805	0.76
hon_000_29071	Ru ₂ Si ₃ Zr	6	-7.203	-7.649	-3.000e-06	0.00639	0.563	0.605
hon_000_29077	Co ₂ Ga ₂ Si ₂	6	-4.872	-5.262	-1.000e-06	0.00485	0.923	2.028
hon_000_29096	GaNd ₂ PbSrYb	6	-3.207	-3.329	-1.000e-06	0.0046	0.421	1.776
hon_000_29100	AlCoGaGeNi ₂	6	-5.011	-5.075	-1.000e-06	0.00751	0.203	0.838
hon_000_29103	AsGeNd ₂ Te ₄	8	-3.775	-4.615	-1.000e-06	0.00631	1.043	4.006
hon_000_29114	GaGd ₄ Na	6	-3.595	-3.712	-1.000e-06	0.00424	0.331	0.379
hon_000_29121	BrCl ₃ IrTb ₂	7	-3.914	-4.853	0.000e+00	0.0044	1.442	2.243
hon_000_29135	Gd ₂ Ir ₂ Se ₄	8	-5.325	-5.964	-3.000e-06	0.00929	1.449	1.927
hon_000_29150	Co ₂ Ga ₃ Pt	6	-4.804	-5.0	0.000e+00	0.00854	0.71	0.569
hon_000_29161	BrNd ₂ SiSn	5	-3.889	-4.898	-3.000e-06	0.00675	1.916	2.295
hon_000_29170	Dy ₂ MgSn ₃	6	-3.958	-4.12	0.000e+00	0.00725	0.428	1.301
hon_000_29175	Dy ₂ GdMgNaPb	6	-3.272	-3.361	-8.000e-06	0.00407	0.4	1.21
hon_000_29192	AsCo ₄ Ge	6	-5.907	-6.17	0.000e+00	0.0078	0.896	2.477
hon_000_29234	AlDy ₂ Sn ₅	8	-3.756	-4.333	-3.000e-06	0.00704	0.788	0.894
hon_000_29268	Sn ₃ Tb ₃	6	-4.27	-4.84	-2.000e-06	0.00439	1.323	1.048
hon_000_29280	GaGd ₂ GeNi ₂	6	-4.918	-5.098	0.000e+00	0.00566	0.59	1.876
hon_000_29301	CrGeNi ₄	6	-5.961	-6.042	-1.300e-05	0.00704	0.423	1.184
hon_000_29323	K ₄ Yb ₂	6	-0.65	-1.017	-1.200e-06	0.00548	1.128	0.922
hon_000_29325	HgIrSnTb ₂ Tl	6	-4.023	-4.489	-5.000e-06	0.00576	1.174	1.19
hon_000_29332	GdGeSnTb ₃	6	-4.483	-4.85	-1.300e-05	0.0069	0.564	1.413
hon_000_29333	Tb ₂ Tl ₄	6	-2.944	-3.244	-1.300e-05	0.00376	1.487	0.82
hon_000_29339	Dy ₂ K ₄	6	-1.513	-1.689	-5.000e-06	0.00448	0.899	2.065
hon_000_29345	Pt ₂ Ru ₂ Zr ₂	6	-8.024	-8.452	-5.000e-06	0.0063	0.924	1.673
hon_000_29347	Li ₂ Ni ₂ SnTi	6	-4.468	-4.711	-1.200e-05	0.00625	0.195	1.895
hon_000_29380	NaSn ₃ Yb ₂	6	-2.652	-2.96	-6.000e-06	0.00509	0.709	1.625
hon_000_29394	Mn ₂ Si ₄	6	-6.494	-6.724	-1.000e-06	0.0062	0.708	1.374
hon_000_29416	Nd ₂ Sn ₄	6	-4.3	-4.703	-2.000e-06	0.00464	1.536	2.818
hon_000_29417	Gd ₄ MgSr	6	-3.382	-3.456	-4.000e-06	0.00448	0.241	0.355
hon_000_29442	AlMn ₂ SbTh	5	-3.998	-6.712	-6.000e-06	0.00658	0.867	1.469
hon_000_29444	CoFe ₂ Sn ₄ Tm	8	-4.845	-5.278	-4.000e-06	0.00616	0.864	0.621
hon_000_29458	DyGa ₂ Ru ₂ Sn	6	-5.265	-5.703	-2.000e-06	0.00539	0.45	0.857
hon_000_29464	CaGd ₃ SrTl	6	-3.138	-3.226	-2.000e-06	0.0046	0.628	1.519
hon_000_29468	Ga ₂ Mn ₂ NiZr	6	-6.243	-6.409	-1.000e-06	0.00381	0.858	0.58

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_29475	AlCrGeNi ₂ Tc	6	-6.511	-6.578	-2.000e-06	0.00784	0.113	0.854
hon_000_29491	Mg ₃ Nd ₃	6	-3.023	-3.155	-1.000e-05	0.00405	1.638	1.698
hon_000_29512	Cs ₃ NaYb ₂	6	-0.901	-0.949	1.000e-07	0.00395	0.557	0.598
hon_000_29520	Fe ₃ Si ₃	6	-6.896	-7.142	0.000e+00	0.00652	0.41	1.146
hon_000_29548	CaGa ₂ PtRu ₂	6	-5.419	-5.504	-4.000e-06	0.00683	0.139	0.969
hon_000_29611	La ₃ Ru ₂ Sb	6	-5.889	-6.509	0.000e+00	0.00664	1.166	3.452
hon_000_29614	Hg ₃ MgTb ₂	6	-1.868	-2.154	0.000e+00	0.00314	1.251	1.803
hon_000_29620	KNd ₂ Sr ₂ Tl	6	-2.364	-2.489	-1.300e-05	0.00491	1.174	3.23
hon_000_29629	MgSn ₃ Yb ₂	6	-2.726	-3.132	0.000e+00	0.00566	1.091	1.858
hon_000_29654	Fe ₃ Na ₃ Sn ₂	8	-3.965	-4.075	-4.000e-06	0.00472	0.735	1.514
hon_000_29671	Bi ₂ Dy ₄	6	-4.612	-4.839	-1.000e-06	0.0028	0.337	2.202
hon_000_29673	Er ₂ InRu ₂	5	-5.244	-6.16	-2.000e-06	0.00471	1.051	2.467
hon_000_29727	Gd ₂ Sn ₄	6	-4.123	-4.655	1.000e-06	0.00533	1.827	1.754
hon_000_29774	Mn ₂ OsSi ₂ Zr	6	-7.948	-8.289	-1.000e-06	0.00513	0.482	1.183
hon_000_29778	Ga ₄ Tb ₂	6	-3.311	-3.742	1.000e-06	0.00867	0.682	2.319
hon_000_29796	AlDy ₃ Ga ₂ Ru	7	-4.584	-5.045	-1.000e-06	0.00438	1.16	0.969
hon_000_29817	GePr ₂ PtRu ₂ Sn	7	-6.106	-6.348	-2.000e-06	0.0052	0.767	2.062
hon_000_29829	NaTl ₃ Yb ₂	6	-1.911	-2.167	0.000e+00	0.00596	2.17	2.543
hon_000_29851	Cd ₂ Tb ₂	4	-2.241	-2.761	0.000e+00	0.00202	0.912	0.793
hon_000_29875	CoNi ₂ Ti ₃	6	-6.999	-7.161	2.500e-05	0.00933	0.376	0.229
hon_000_29877	AgAlMg ₂ Ru ₂ Tb	7	-4.526	-4.68	-6.000e-06	0.00507	0.481	1.211
hon_000_29889	Co ₃ Gd ₂ Ge	6	-5.951	-6.126	-2.000e-06	0.00935	0.485	2.291
hon_000_29895	AlFe ₃ Pt	5	-6.576	-6.674	-5.000e-06	0.00794	0.307	1.939
hon_000_29939	LaNaSrThYb ₂	6	-2.704	-2.79	-5.000e-06	0.0077	0.834	1.828
hon_000_29941	Fe ₂ Li ₂ Si ₃ W	8	-5.942	-6.187	1.300e-05	0.00563	0.588	1.167
hon_000_30006	BrNd ₂ PbSr	5	-3.247	-3.895	-1.000e-06	0.00325	1.756	1.484
hon_000_30009	AlGaMn ₂ Sn	5	-5.048	-5.461	0.000e+00	0.00211	0.771	0.585
hon_000_30024	HoNd ₂ Pb ₂ Sn	6	-4.29	-4.662	0.000e+00	0.00918	1.493	1.409
hon_000_30054	Ge ₅ Ni ₂ Pt	8	-4.535	-4.985	-2.000e-06	0.00747	0.85	1.028
hon_000_30070	Ca ₂ Co ₂ CuGa	6	-3.975	-4.057	1.000e-06	0.00443	0.539	0.507
hon_000_30089	AlLiMoNi ₂ Si	6	-5.557	-5.665	-2.000e-06	0.00717	0.341	2.447
hon_000_30133	Br ₃ ClGd ₂ Ru	7	-3.737	-4.864	-4.000e-06	0.00719	1.863	2.57
hon_000_30150	Al ₂ Co ₃ Ge	6	-5.462	-5.732	-7.000e-06	0.00727	0.162	0.41
hon_000_30153	Cd ₂ La ₂ Ru ₂	6	-4.864	-5.045	0.000e+00	0.00446	0.497	1.881
hon_000_30164	B ₂ Mn ₂ Pt ₃	7	-6.326	-7.057	-4.000e-05	0.00968	0.32	1.766
hon_000_30169	AlFe ₂ Pt ₂ Zr ₂	7	-7.277	-7.515	-1.200e-05	0.00888	0.281	1.502
hon_000_30255	MgSn ₂ TlYb ₂	6	-2.426	-2.803	0.000e+00	0.00697	1.074	4.217
hon_000_30273	Br ₄ Gd ₂ Rh	7	-3.73	-4.488	-1.000e-06	0.00503	1.719	3.372
hon_000_30293	Mn ₂ SiV ₃	6	-8.471	-8.688	3.000e-06	0.00528	0.614	1.219
hon_000_30321	Ga ₂ Gd ₂ Sr	5	-2.94	-3.698	2.000e-06	0.00519	1.18	2.586
hon_000_30372	GaLu ₂ Ru ₂ Tl	6	-4.976	-5.579	0.000e+00	0.00629	0.7	2.207
hon_000_30384	GaLu ₂ PbRu ₂	6	-5.147	-5.816	-7.000e-06	0.0066	1.264	1.997
hon_000_30403	Dy ₂ Eu ₃ In	6	-2.843	-2.961	0.000e+00	0.00535	0.446	0.558
hon_000_30408	Co ₃ Li ₃	6	-4.24	-4.27	0.000e+00	0.0025	0.136	0.85
hon_000_30422	AlDy ₃ MgSn ₂	7	-3.676	-4.111	-1.000e-06	0.00525	0.918	0.999
hon_000_30450	Dy ₂ PbRb ₅	8	-1.65	-1.715	-3.000e-06	0.00298	0.789	2.263
hon_000_30458	Gd ₃ Li ₂ Zn	6	-2.936	-3.038	-1.000e-06	0.00668	0.451	0.308
hon_000_30470	Cl ₄ PtYb ₂	7	-3.034	-4.141	1.000e-06	0.00499	1.405	3.503
hon_000_30486	Au ₂ Mn ₂	4	-5.173	-5.663	-6.200e-05	0.00373	0.796	0.636
hon_000_30491	Sn ₄ Yb ₂	6	-3.198	-3.455	1.000e-06	0.00269	0.678	1.42
hon_000_30493	Cr ₂ GeNi ₂ Si	6	-6.495	-6.581	-4.000e-06	0.00823	0.232	0.771
hon_000_30499	Gd ₂ Se ₄ Sn ₂	8	-3.758	-4.978	-2.000e-06	0.00712	0.996	2.535

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_30510	Co ₃ Pd ₂ Ti	6	-6.459	-6.633	-3.000e-06	0.00477	0.555	1.784
hon_000_30512	AlMn ₃ Pt ₂	6	-6.959	-7.42	-1.000e-05	0.00723	0.595	0.516
hon_000_30523	Cs ₄ Yb ₂	6	-0.702	-0.837	1.000e-07	0.00242	0.925	0.557
hon_000_30529	Gd ₆	6	-4.548	-4.581	-3.000e-06	0.00292	0.176	0.241
hon_000_30563	Al ₂ MgPr ₂ Ru ₂	7	-5.07	-5.198	3.000e-06	0.00799	0.614	1.912
hon_000_30580	Sn ₄ Yb ₂	6	-3.192	-3.455	-7.000e-06	0.00623	0.882	0.372
hon_000_30590	AuMg ₂ Ni ₃	6	-3.812	-3.886	-1.500e-05	0.00999	0.355	1.862
hon_000_30604	Na ₂ Yb ₄	6	-1.235	-1.353	1.500e-06	0.00361	0.943	1.199
hon_000_30609	AlAsNdNi ₂	5	-4.908	-5.148	-9.300e-05	0.00488	0.417	2.424
hon_000_30640	Co ₂ Pt ₃ Sn ₃	8	-5.476	-5.64	-1.000e-06	0.00764	0.772	1.866
hon_000_30650	CdInMgPbYb ₂	6	-2.093	-2.151	-5.000e-06	0.00663	0.638	0.665
hon_000_30668	Cs ₄ Yb ₂	6	-0.736	-0.837	-1.700e-06	0.0027	0.709	1.64
hon_000_30717	AgGaPr ₂ Ru ₂	6	-5.185	-5.768	0.000e+00	0.00829	0.821	1.433
hon_000_30721	Co ₂ GaLi ₂	5	-3.792	-4.121	2.000e-06	0.00372	0.945	1.657
hon_000_30729	LiPd ₃ Ru ₂	6	-5.851	-5.898	6.000e-06	0.00863	0.232	0.188
hon_000_30747	Fe ₂ Ge ₂ Ni ₂	6	-5.394	-6.002	-5.000e-06	0.00647	0.666	1.145
hon_000_30760	AlCo ₂ Sc ₃	6	-6.045	-6.332	-1.000e-06	0.00542	1.086	1.451
hon_000_30805	CaCo ₂ GaSb	5	-4.246	-4.681	-3.000e-06	0.00624	1.224	2.335
hon_000_30806	Gd ₂ SSe ₃ W ₂	8	-5.986	-6.906	0.000e+00	0.00472	1.562	3.438
hon_000_30812	Dy ₂ K ₄	6	-1.587	-1.67	-1.400e-05	0.00541	0.592	1.291
hon_000_30815	Br ₂ I ₂ Yb ₂	6	-2.208	-3.3	-1.000e-06	0.00533	4.071	3.608
hon_000_30825	CoHfNi ₂ Sn	5	-6.289	-6.541	-4.000e-06	0.00661	0.309	0.46
hon_000_30853	NdTb ₄ Y	6	-4.765	-4.886	-2.000e-06	0.00215	0.875	1.625
hon_000_30877	GaGeSb ₂ Tb ₄	8	-4.224	-5.013	-1.000e-06	0.00463	0.885	1.425
hon_000_30885	Rh ₂ Sn ₂ Tb ₂ Th ₂	8	-6.208	-6.381	0.000e+00	0.00354	0.556	0.904
hon_000_30899	Co ₂ Fe ₂ Ge ₂	6	-6.306	-6.456	0.000e+00	0.00454	0.501	1.453
hon_000_30919	GdPb ₂ SrTb ₂	6	-3.647	-3.987	-9.000e-06	0.0054	0.778	2.277
hon_000_30973	MnNi ₄ Si	6	-5.914	-6.187	-9.000e-06	0.00506	0.275	0.967
hon_000_30986	MgNa ₂ Nd ₂ Pb	6	-2.613	-2.924	-1.000e-06	0.0037	1.778	2.371
hon_000_30988	AgAuBiEr ₂ Ru ₂	7	-5.337	-5.478	-4.000e-06	0.00761	0.705	1.856
hon_000_30995	AlCo ₃ ErGaNd	7	-4.906	-5.383	-6.000e-06	0.00578	0.981	0.841
hon_000_31005	Gd ₂ RhSe ₄	7	-4.745	-5.638	2.000e-06	0.00581	1.494	1.651
hon_000_31020	Fe ₂ Ga ₃ La	6	-4.859	-5.165	-2.000e-06	0.00309	0.475	1.21
hon_000_31030	FeGd ₄ NiSr ₂	8	-4.147	-4.288	-1.000e-06	0.0051	0.437	0.359
hon_000_31031	BiDy ₅	6	-4.561	-4.621	-2.000e-05	0.0054	0.795	0.351
hon_000_31046	Al ₂ GaGdNi ₂	6	-4.464	-4.804	-1.000e-06	0.00652	0.336	1.534
hon_000_31049	Br ₄ PtTb ₂	7	-3.521	-4.583	-1.000e-06	0.00764	1.53	3.788
hon_000_31050	Na ₃ SnYb ₂	6	-1.766	-1.902	-3.000e-06	0.00495	1.144	3.107
hon_000_31058	Ni ₂ Y ₂ Zn ₂	6	-4.652	-4.698	-5.000e-06	0.00747	0.292	0.88
hon_000_31061	In ₃ Lu ₂ PdRu ₂	8	-4.924	-5.309	-1.300e-05	0.0073	0.705	0.493
hon_000_31083	CaFe ₂ SiSn	5	-4.625	-5.5	-5.000e-06	0.00533	1.061	1.662
hon_000_31101	Fe ₃ SiV ₂	6	-8.127	-8.261	-1.000e-05	0.00453	0.355	1.01
hon_000_31115	AlMn ₂ Mo ₃ Ni ₂	8	-7.725	-8.046	-1.000e-05	0.00883	0.276	1.371
hon_000_31124	CuGaNi ₂ U ₂	6	-6.658	-6.753	-1.000e-06	0.0045	0.214	0.9
hon_000_31146	Co ₂ Si ₄	6	-5.77	-6.065	-3.000e-06	0.00798	0.621	0.604
hon_000_31208	CdDy ₃ Pt ₂ SbSi	8	-4.948	-5.356	1.000e-06	0.00489	1.642	1.707
hon_000_31217	AlGdNi ₂ P	5	-4.992	-5.369	-6.000e-06	0.00906	0.598	1.36
hon_000_31246	Al ₂ BePdRu ₂	6	-5.655	-6.213	-1.000e-06	0.00426	0.725	0.495
hon_000_31267	Nd ₃ Zn ₅	8	-2.428	-2.729	-1.700e-05	0.00672	0.631	2.973
hon_000_31322	AlCo ₂ MgSi ₂	6	-4.868	-5.36	-1.000e-06	0.00782	0.885	1.542
hon_000_31330	MgNd ₂ Sn ₃	6	-3.982	-4.262	-1.000e-06	0.00308	1.664	0.773
hon_000_31340	Nd ₂ Sr ₄	6	-2.361	-2.479	-1.500e-05	0.0026	0.391	0.502

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
hon_000_31342	Al ₂ Fe ₃ Gd ₂	7	-5.635	-5.934	-1.600e-05	0.00533	0.637	1.572
hon_000_31343	Al ₂ Ni ₃ Si ₂ Th	8	-5.624	-5.845	4.000e-06	0.00954	1.025	2.515
hon_000_31346	AlCo ₂ Dy ₂ Fe	6	-5.665	-5.913	2.000e-06	0.00505	0.636	2.1
hon_000_31364	Nd ₂ Pd ₂ Se ₄	8	-4.63	-5.369	0.000e+00	0.00612	2.232	1.852
hon_000_31386	Er ₂ GaRu ₂ Sb	6	-5.75	-5.987	-1.000e-05	0.00931	0.493	0.383
hon_000_31441	Co ₂ PdPtSnY	6	-6.069	-6.233	-3.000e-06	0.00923	0.634	0.6
hon_000_31455	AlNi ₃ Ti ₂	6	-6.32	-6.418	-1.000e-06	0.00676	1.056	2.07
hon_000_31465	Al ₂ Co ₂ GeLi	6	-4.566	-4.717	-1.000e-06	0.00421	0.599	1.209
hon_000_31482	Mn ₂ Si ₃	5	-6.524	-6.892	-7.000e-06	0.00607	0.769	2.201
hon_000_31500	CoRu ₂ Sb ₂ Th ₂	7	-7.13	-7.353	-4.600e-05	0.00918	0.648	1.287
hon_000_31502	Co ₂ Ga ₄	6	-4.091	-4.297	-2.000e-06	0.00415	0.71	1.151
hon_000_31503	AlDyGaRu ₂ Si ₃	8	-5.646	-6.088	-1.000e-06	0.00704	0.963	1.409
hon_000_31539	Fe ₂ Ga ₄	6	-4.428	-4.624	0.000e+00	0.00862	0.73	2.154
hon_000_31570	K ₂ Pb ₃ SbYb ₂	8	-2.556	-2.736	5.000e-06	0.00661	0.791	1.599
hon_000_31582	AlMn ₂ NiPtSi	6	-6.543	-6.744	1.000e-06	0.0074	0.369	0.98
hon_000_31594	HFe ₂ NaSn	5	-4.012	-4.546	-4.000e-06	0.00955	1.269	2.049
hon_000_31641	Au ₂ Gd ₂ Tl ₂	6	-3.275	-3.818	-4.000e-06	0.00491	1.153	2.552
hon_000_31672	GeMg ₂ Mn ₂ Y	6	-4.655	-5.216	-2.000e-06	0.00371	0.901	2.583
hon_000_31682	Ca ₂ Co ₂ PtSi	6	-4.993	-5.182	1.300e-05	0.00458	0.587	1.88
hon_000_31698	Ga ₄ Tb ₂	6	-3.371	-3.987	0.000e+00	0.00784	1.532	2.144
hon_000_31716	Li ₃ Mg ₃ Ni ₂	8	-2.416	-2.584	-1.000e-05	0.00378	0.762	2.529
hon_000_31743	Ga ₄ Mn ₂	6	-4.655	-4.844	-2.000e-06	0.00778	0.578	1.289
hon_000_31748	AlPr ₂ Ru ₂ Sn	6	-5.8	-6.146	-2.000e-06	0.00729	0.747	2.229
hon_000_31760	CdRu ₂ Tm ₃	6	-5.322	-5.449	0.000e+00	0.0057	0.55	1.118
hon_000_31765	Cl ₄ Pt ₂ Tb ₂	8	-4.02	-4.901	0.000e+00	0.0087	1.737	2.835
hon_000_31776	DyRu ₅	6	-8.187	-8.297	2.000e-06	0.00509	0.439	0.435
hon_000_31794	AlCe ₃ Ru ₂	6	-6.491	-7.0	-4.000e-06	0.00589	0.897	1.242
hon_000_31795	CaNa ₃ Yb ₂	6	-1.332	-1.38	-3.400e-06	0.0057	0.94	1.625
hon_000_31823	CaMgSn ₂ Yb ₂	6	-2.484	-2.638	0.000e+00	0.00861	0.705	0.75
hon_000_31845	BaNaPbYb ₂	5	-1.629	-2.074	-4.000e-06	0.00737	2.385	2.257
hon_000_31847	AlGaHfMn ₂	5	-6.384	-7.026	2.000e-06	0.00632	0.972	0.703
hon_000_31854	Co ₃ Si ₃	6	-6.014	-6.603	-6.200e-05	0.00646	0.492	1.771
hon_000_31861	Au ₃ Fe ₂ Ga	6	-4.415	-4.546	-2.000e-06	0.00286	0.794	1.964
hon_000_31885	Ni ₄ Sn	5	-4.939	-5.141	-1.000e-06	0.00374	0.568	1.286
hon_000_31887	Nd ₂ Sn ₃	5	-4.103	-4.745	-5.000e-06	0.0046	1.493	1.074
hon_000_31901	As ₃ CdMn ₂ Nd ₂	8	-4.881	-5.595	-8.000e-06	0.00513	1.004	2.036
hon_000_31916	CaEu ₂ Yb ₃	6	-1.616	-1.667	0.000e+00	0.0041	0.423	0.279
hon_000_31927	Li ₂ N ₂ Sn ₂ Tb ₂	8	-4.847	-5.069	-2.000e-06	0.00404	0.487	1.948
hon_000_31967	BiDy ₂ Rb ₅	8	-1.902	-1.916	2.000e-06	0.00627	0.649	1.561
hon_000_31972	Sn ₄ Yb ₂	6	-3.197	-3.455	2.000e-06	0.00802	0.85	1.38
hon_000_31979	Sn ₄ Yb ₂	6	-3.061	-3.458	-2.300e-05	0.00513	0.756	0.678
hon_000_31997	Be ₂ Ni ₂ RhSn	6	-4.684	-5.11	-6.000e-06	0.00581	0.883	1.77
hon_000_32004	Fe ₂ Ho ₂ RuSn	6	-6.257	-6.446	0.000e+00	0.00515	0.585	3.026
hon_000_32011	AlAuMn ₂ Rh ₂	6	-6.434	-6.633	-8.000e-06	0.00535	0.272	0.262
hon_000_32016	Ga ₂ Gd ₂ PdTl ₃	8	-3.336	-3.695	-4.000e-06	0.0051	1.611	0.911
hon_000_32017	Cl ₄ Dy ₂ Pt	7	-3.697	-4.564	-5.000e-06	0.00712	0.905	2.828
hon_000_32019	Ga ₃ SnYb ₂	6	-2.461	-3.056	3.000e-06	0.00732	2.079	2.658
hon_000_32066	CaGa ₃ Gd ₂ Ir	7	-4.09	-4.564	-1.000e-06	0.00563	0.832	2.315
hon_000_32098	Ce ₃ Dy ₂ Tl	6	-4.575	-4.891	6.000e-06	0.00788	1.398	2.868
hon_000_32148	Gd ₃ HoSn ₂	6	-4.503	-4.764	-1.000e-06	0.00674	1.779	1.254
hon_000_32153	La ₃ Nd ₂ Sr	6	-4.085	-4.186	-1.300e-05	0.00439	0.657	1.57
hon_000_32187	CaNa ₂ Nd ₂ Sr	6	-2.404	-2.399	-4.000e-06	0.00337	0.162	1.301

Table S5. The profile of generated materials with Honeycomb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E_{start}	E_{final}	E_{conv}	F_{max}	d_{latt}	d_{xy}
hon_000_32208	Br ₄ Ir ₂ Yb ₂	8	-3.504	-4.075	1.900e-05	0.00989	1.77	4.645
hon_000_32224	AlAsNa ₂ PbTb ₂	7	-3.353	-3.754	-9.000e-06	0.00453	0.995	1.033
hon_000_32250	Mn ₂ ScSi ₂	5	-6.732	-7.194	-2.000e-06	0.0056	1.091	1.789
hon_000_32256	Dy ₂ I ₄ Ru ₂	8	-4.035	-4.432	3.000e-06	0.00857	0.993	1.708
hon_000_32258	Au ₃ MnRu ₂	6	-5.228	-5.842	-1.300e-05	0.00938	1.009	1.652
hon_000_32262	MgNa ₂ Nd ₂ Sn	6	-2.874	-3.013	-1.400e-05	0.00565	0.603	1.376
hon_000_32266	Gd ₂ Hf ₂ MgSn	6	-5.387	-5.729	0.000e+00	0.0039	0.481	1.568
hon_000_32270	Ga ₂ Gd ₂ Sr ₂	6	-2.864	-3.288	-1.000e-06	0.00218	1.013	1.836
hon_000_32328	Tl ₄ Yb ₂	6	-2.111	-2.25	2.000e-06	0.00173	0.849	1.636

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation

Index	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_00029	CaLaSn ₃ Tb ₃	8	-4.216	-4.477	-1.000e-06	0.00895	0.663	0.631
kag_000_00057	AlEuIn ₂ PtTb ₃	8	-3.853	-4.323	-3.000e-06	0.00915	1.254	1.428
kag_000_00076	Ca ₃ Gd ₃ MgNa	8	-2.601	-2.663	-1.000e-06	0.00403	0.544	2.921
kag_000_00092	Dy ₃ Na ₄ Sn	8	-2.669	-2.733	-3.000e-06	0.00609	1.311	2.419
kag_000_00096	Dy ₂ FeNi ₃	6	-5.872	-5.891	0.000e+00	0.00524	0.119	0.065
kag_000_00099	Al ₂ Ni ₃ Ru ₃ Zr ₄	12	-7.494	-7.655	2.000e-06	0.00752	0.413	0.514
kag_000_00119	Na ₅ Yb ₃	8	-1.283	-1.286	-1.000e-06	0.00213	0.177	0.121
kag_000_00128	Ni ₅ Pt ₃	8	-5.477	-5.747	-8.000e-06	0.00641	0.571	1.545
kag_000_00141	Dy ₃ Tl ₅	8	-3.184	-3.29	-1.000e-06	0.00635	0.989	0.836
kag_000_00166	BaDy ₃ HgKNa	7	-2.106	-2.349	0.000e+00	0.00367	1.628	1.341
kag_000_00174	BaBrGd ₃ ISnTl	8	-3.08	-3.861	-1.000e-06	0.00489	2.16	3.008
kag_000_00207	Al ₃ Ni ₅	8	-5.234	-5.355	-2.000e-06	0.00813	0.46	0.27
kag_000_00228	Ge ₂ Hf ₃ MoNi ₅	11	-7.147	-7.435	-1.700e-05	0.00657	0.467	0.561
kag_000_00240	ErGeNi ₃ Pt ₃	8	-5.641	-5.832	3.000e-06	0.00946	1.063	0.768
kag_000_00253	Sn ₂ Yb ₆	8	-2.18	-2.519	0.000e+00	0.00512	2.006	1.705
kag_000_00254	Mn ₄ Pt ₄	8	-7.262	-7.567	-1.200e-05	0.00575	0.417	0.365
kag_000_00259	AsNi ₃ Se ₂ Zn ₂	8	-3.432	-3.907	-1.000e-06	0.00674	1.33	2.196
kag_000_00290	Dy ₃ In ₅	8	-3.788	-3.614	-3.000e-06	0.00655	0.619	1.152
kag_000_00332	AlNi ₆	7	-5.222	-5.266	0.000e+00	0.00992	0.229	0.145
kag_000_00338	Co ₆ Ni ₂	8	-6.362	-6.435	1.100e-05	0.00635	0.149	0.126
kag_000_00358	AlCaDy ₃ GeLa ₅ Sr	12	-4.048	-4.233	-1.000e-06	0.00457	2.077	1.95
kag_000_00431	MnNi ₁₁	12	-5.58	-5.706	4.000e-06	0.00439	0.291	0.293
kag_000_00442	Na ₃ SrTiYb ₃	8	-1.457	-1.555	0.000e+00	0.00914	0.98	1.078
kag_000_00449	Co ₄ Dy ₂	6	-6.316	-6.381	-1.110e-04	0.00752	0.147	0.184
kag_000_00470	AgLaNa ₂ Tb ₃ Tl	8	-3.02	-3.251	-1.000e-06	0.00643	1.953	0.994
kag_000_00471	GaPt ₃ Ru ₃ Zr	8	-7.408	-7.499	-6.000e-06	0.00533	0.154	0.172
kag_000_00503	CoCs ₂ Dy ₃ Fe ₂ Se ₃	11	-4.293	-4.765	1.000e-05	0.00625	1.327	2.488
kag_000_00512	Al ₂ Fe ₅ Pt	8	-6.666	-6.902	-4.700e-05	0.00475	0.967	1.699
kag_000_00514	CdTl ₂ Yb ₅	8	-1.665	-1.885	-1.100e-05	0.00464	1.076	1.295
kag_000_00518	Co ₃ Ga ₃ GeNiSn ₄	12	-3.997	-4.51	-1.000e-06	0.00899	0.915	1.784
kag_000_00521	Fe ₆ Si ₂ Ta ₄	12	-9.226	-9.356	0.000e+00	0.00845	0.238	0.241
kag_000_00525	AuCo ₃ Ga ₂ Sc	7	-5.145	-5.347	-1.000e-06	0.00746	0.466	0.904
kag_000_00564	Al ₃ Co ₃ Zr	7	-5.971	-6.069	0.000e+00	0.00747	0.324	0.379
kag_000_00566	Dy ₄ GaN ₂ Sr	8	-2.852	-2.999	0.000e+00	0.00615	0.656	3.2
kag_000_00573	Pt ₅ Ru ₃	8	-6.761	-7.189	1.000e-06	0.0075	0.699	0.537
kag_000_00586	Dy ₃ I ₃ RhTl ₂	9	-3.36	-3.877	0.000e+00	0.00312	1.786	2.765
kag_000_00590	EuNa ₃ Yb ₄	8	-1.345	-1.379	0.000e+00	0.00224	0.68	2.186
kag_000_00603	I ₅ Nd ₃ Si	9	-3.115	-3.976	0.000e+00	0.00418	2.369	3.216
kag_000_00610	GaLuSb ₂ Tb ₄	8	-4.548	-4.714	-1.100e-05	0.0051	0.61	0.358
kag_000_00630	Dy ₃ LaNaS ₆	11	-5.476	-5.82	-6.000e-06	0.0085	1.164	1.142
kag_000_00645	Na ₄ TiYb ₃	8	-1.439	-1.458	-2.000e-06	0.00386	0.549	2.126
kag_000_00652	Mn ₄ Pt ₂ SiTc	8	-8.001	-8.06	-1.000e-06	0.00675	0.213	1.523
kag_000_00653	Co ₄ Fe ₄	8	-7.372	-7.462	-1.000e-06	0.00732	0.175	0.718
kag_000_00675	AlBNiPrRu ₅	9	-7.249	-7.399	-3.000e-06	0.00791	0.357	1.573
kag_000_00682	InNa ₄ Tb ₃	8	-2.597	-2.586	-2.000e-06	0.00429	0.579	2.016
kag_000_00687	Al ₂ ErMn ₃	6	-6.049	-6.357	-8.000e-06	0.00765	0.516	0.613
kag_000_00688	Cl ₅ Mn ₂ Tb ₃	10	-4.362	-5.071	-1.000e-06	0.00714	1.366	4.115
kag_000_00710	Fe ₄ Y ₂	6	-7.527	-7.552	-1.500e-05	0.00717	0.071	0.94
kag_000_00735	EuInNa ₂ Yb ₄	8	-1.581	-1.645	-7.500e-05	0.0081	0.84	0.432
kag_000_00741	AlFe ₄ Pt ₃	8	-6.811	-6.881	-3.000e-06	0.00925	0.184	0.822
kag_000_00747	Ca ₂ Dy ₃ Na ₃	8	-2.431	-2.439	-7.000e-06	0.00302	0.175	1.015
kag_000_00750	La ₂ Ni ₄	6	-5.496	-5.59	-5.000e-06	0.00588	0.189	0.159

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_00762	GeMn ₄ U ₂	7	-8.886	-9.129	-2.000e-06	0.00931	0.325	0.453
kag_000_00778	Dy ₅ EuNa ₂	8	-3.134	-3.154	-2.200e-05	0.00645	1.161	2.18
kag_000_00807	AlCo ₇	8	-6.449	-6.615	-6.300e-05	0.00654	0.572	0.375
kag_000_00830	Co ₄ Ga ₂ Ge ₂	8	-5.253	-5.342	-1.000e-06	0.0058	0.362	0.183
kag_000_00863	AlGaNi ₃ PtUZr	8	-5.974	-6.419	-5.000e-06	0.00425	0.739	1.449
kag_000_00903	CrMn ₃ Ni ₄	8	-7.025	-7.206	-4.100e-05	0.00585	0.215	0.137
kag_000_00916	Al ₄ CaNd ₃ Ru	9	-4.311	-4.706	-1.100e-05	0.00815	1.092	2.32
kag_000_00935	Br ₃ IND ₃ PRb	9	-3.013	-4.14	-1.000e-06	0.00643	2.408	2.408
kag_000_00936	NdNi ₃ SmSn ₂	7	-4.94	-5.029	3.000e-06	0.00823	0.67	0.591
kag_000_00957	Ni ₃ SSnSr ₂	7	-3.518	-4.401	1.000e-06	0.00833	1.189	2.065
kag_000_00973	Co ₃ Fe ₅	8	-7.389	-7.619	0.000e+00	0.00295	0.251	0.221
kag_000_00975	FeGa ₂ Mn ₇ Zr ₂	12	-7.509	-7.891	-7.000e-06	0.0039	0.575	0.498
kag_000_00980	Ni ₆ Sn ₅ Yb	12	-4.374	-4.663	-4.000e-06	0.00673	0.258	0.887
kag_000_01045	MgNi ₈ Ta ₂ V	12	-6.454	-6.635	-1.000e-06	0.00713	0.51	0.612
kag_000_01049	Dy ₃ Na ₄ Sn	8	-2.669	-2.729	-4.000e-06	0.0035	0.841	1.421
kag_000_01058	Dy ₃ Na ₅	8	-2.189	-2.216	0.000e+00	0.0053	0.832	2.325
kag_000_01071	Fe ₃ GaNi ₄	8	-5.757	-6.125	-6.000e-06	0.00432	0.726	0.576
kag_000_01073	GdSrTb ₃ Yb ₃	8	-2.808	-2.871	-1.600e-05	0.00297	0.584	1.348
kag_000_01143	Na ₅ Yb ₃	8	-1.248	-1.286	2.000e-06	0.00466	0.162	1.436
kag_000_01159	Fe ₃ SiY ₂	6	-7.107	-7.351	-7.400e-05	0.00912	0.353	1.09
kag_000_01168	AsGe ₂ Mn ₄ Ti	8	-7.046	-7.223	0.000e+00	0.00794	0.397	2.201
kag_000_01172	Br ₈ CdNd ₃	12	-3.794	-3.892	0.000e+00	0.00622	0.583	2.39
kag_000_01199	Dy ₃ Na ₄ Sr	8	-2.252	-2.264	2.000e-06	0.00177	0.324	0.331
kag_000_01216	Co ₅ Ni ₂ Pt	8	-6.253	-6.356	-1.400e-05	0.00335	0.31	0.175
kag_000_01231	CoPt ₃ Ru ₄	8	-7.107	-7.645	4.000e-06	0.00521	0.234	0.227
kag_000_01254	ClDy ₃ PbTl	6	-3.404	-4.176	0.000e+00	0.00783	2.328	2.9
kag_000_01255	Na ₅ Tb ₃	8	-2.203	-2.236	-4.000e-06	0.00484	0.335	0.21
kag_000_01276	BaInLuSnSrTb ₃	8	-3.522	-3.622	-5.000e-06	0.00997	1.473	2.0
kag_000_01304	Fe ₆ Ni ₂	8	-7.122	-7.349	-6.000e-06	0.00492	0.373	0.194
kag_000_01307	Co ₃ GeNi ₂ TcTi	8	-6.768	-6.941	-3.400e-05	0.00743	0.67	1.147
kag_000_01346	BaGd ₃ Na ₄	8	-2.259	-2.302	-7.000e-06	0.00317	0.258	0.18
kag_000_01360	FeRh ₄ Ru ₃	8	-7.851	-8.043	-1.000e-05	0.00752	0.263	0.131
kag_000_01362	AlPd ₄ Yb ₇	12	-3.425	-3.52	-4.400e-05	0.00593	0.78	1.339
kag_000_01366	CeGa ₄ Tb ₃	8	-4.007	-4.233	-4.000e-06	0.00945	0.561	0.484
kag_000_01384	CaEuTb ₃ Tl ₃	8	-3.128	-3.263	-1.000e-06	0.00559	0.523	1.382
kag_000_01443	EuNa ₄ Yb ₃	8	-1.345	-1.354	2.000e-06	0.00977	0.181	0.223
kag_000_01473	Co ₅ Ga ₂ Re	8	-6.412	-6.571	-1.000e-06	0.0092	0.447	0.316
kag_000_01514	Ni ₈ ZnZr ₂	11	-5.628	-5.83	2.000e-06	0.00504	0.449	0.293
kag_000_01517	GeNi ₅ PtZn	8	-4.842	-5.099	-2.700e-05	0.00403	0.434	0.269
kag_000_01527	GeRu ₄ SiTcTi	8	-8.119	-8.37	-1.000e-06	0.00505	0.472	2.287
kag_000_01540	Ba ₄ Gd ₃ Tl	8	-2.765	-2.836	-1.000e-05	0.00272	0.265	1.39
kag_000_01554	CrFe ₅ SiZn	8	-6.828	-7.068	-7.000e-06	0.00614	0.85	1.613
kag_000_01575	Na ₄ PbTb ₃	8	-2.594	-2.688	0.000e+00	0.00621	0.894	2.172
kag_000_01580	Mn ₃ RhSe ₈	12	-5.142	-5.338	-5.000e-06	0.00947	0.471	1.455
kag_000_01581	EuINaRhSn ₂ Tb ₃	9	-3.8	-4.178	-1.000e-06	0.00766	1.387	4.461
kag_000_01588	BaCaDy ₃ Eu ₂ Sn	8	-3.063	-3.156	1.000e-06	0.00229	0.492	0.747
kag_000_01596	Co ₄ MoNiVZr ₄	11	-8.029	-8.078	-1.200e-05	0.00524	0.222	0.329
kag_000_01599	Na ₂ Ru ₃ Sn	6	-4.634	-5.342	-9.000e-06	0.00766	0.818	0.567
kag_000_01612	BaNa ₄ Yb ₃	8	-1.263	-1.365	-1.800e-05	0.00383	0.746	3.059
kag_000_01620	Ru ₄ Sb ₂ Zr	7	-7.359	-7.702	-5.000e-06	0.00608	0.418	0.588
kag_000_01649	FeNi ₇	8	-5.67	-5.703	-9.000e-06	0.00585	0.176	0.81
kag_000_01652	LuTl ₄ Yb ₃	8	-2.249	-2.476	-1.800e-05	0.00403	0.734	0.419

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_01664	AgAlCaTb ₃ Zn	7	-2.97	-3.503	0.000e+00	0.0041	2.395	2.941
kag_000_01671	Na ₅ Yb ₃	8	-1.258	-1.285	-1.000e-06	0.00084	0.591	0.562
kag_000_01673	AlFe ₃ PtSi ₂	7	-6.477	-6.722	-6.000e-06	0.00765	0.67	0.542
kag_000_01674	CaCe ₂ EuSnTb ₃	8	-4.171	-4.188	-6.600e-05	0.00804	0.193	0.121
kag_000_01683	In ₃ LuNd ₃ Tl	8	-3.519	-3.883	-2.000e-06	0.00957	1.662	0.969
kag_000_01690	BPtRu ₄ SiTm ₂	9	-7.155	-7.587	-1.000e-05	0.00893	0.435	2.67
kag_000_01750	Er ₂ Fe ₃ Ni	6	-6.542	-6.629	-1.000e-06	0.00603	0.312	1.025
kag_000_01776	AgCo ₄ DyMo	7	-6.086	-6.362	-5.800e-05	0.00753	0.352	0.419
kag_000_01785	FeGa ₃ Ni ₄	8	-4.948	-4.973	-3.300e-05	0.0067	0.195	0.194
kag_000_01798	Br ₂ Dy ₃ Fe ₂ S ₃ V	11	-5.05	-5.787	-3.400e-05	0.00973	1.528	3.556
kag_000_01832	Ca ₂ Co ₃ Mn	6	-4.842	-5.41	-6.000e-06	0.00443	1.168	0.65
kag_000_01848	Ni ₄ Pt ₂ Si ₂	8	-5.467	-5.964	-5.000e-06	0.00895	0.67	0.539
kag_000_01855	AuCdPtRu ₃	6	-5.302	-5.869	-3.000e-06	0.00682	1.212	1.852
kag_000_01862	Eu ₂ MgNd ₅	8	-3.486	-3.554	0.000e+00	0.00353	0.967	2.502
kag_000_01868	BrCaIrLaTb ₃ Tl ₂	9	-4.127	-4.425	8.000e-06	0.00693	0.732	2.739
kag_000_01870	EuIrSn ₂ Yb ₅	9	-3.027	-3.301	-2.600e-05	0.00694	1.833	4.626
kag_000_01879	Na ₄ Nd ₃ Sn	8	-2.822	-2.91	-1.000e-05	0.00416	1.072	3.36
kag_000_01916	LaSrTe ₇ Yb ₃	12	-3.52	-4.03	2.000e-06	0.00438	0.653	2.011
kag_000_01919	Gd ₆ SnTe	8	-4.544	-4.777	-2.000e-06	0.00242	0.531	2.085
kag_000_01947	CaGd ₄ La ₂ Sb	8	-4.291	-4.498	-1.000e-06	0.00248	0.283	1.307
kag_000_01958	AlMn ₃ Na ₂ Pd ₂	8	-5.009	-5.265	9.000e-06	0.00592	0.399	0.325
kag_000_01959	Cd ₂ Tl ₂ Yb ₄	8	-1.511	-1.756	-1.000e-06	0.00305	1.366	2.428
kag_000_01966	CaKNa ₃ Tb ₃	8	-2.163	-2.231	-2.000e-06	0.00112	0.777	1.403
kag_000_02006	Co ₃ Fe ₂ Ni ₃	8	-6.131	-6.554	3.000e-06	0.00433	0.451	0.293
kag_000_02008	Mn ₃ Sn ₃ V	7	-6.143	-6.418	0.000e+00	0.0063	0.522	0.598
kag_000_02012	Ni ₇ Pu	8	-6.377	-6.406	5.000e-06	0.00701	0.225	0.792
kag_000_02020	AuMnSe ₅ Tb ₃ Ti ₂	12	-5.037	-5.829	-1.000e-06	0.00611	2.088	3.564
kag_000_02030	AgAlCe ₂ EuGd ₃ Rh	9	-4.525	-4.731	-1.200e-05	0.00674	1.03	2.467
kag_000_02034	Eu ₂ Tl ₂ Yb ₄	8	-1.86	-2.013	-7.000e-06	0.00418	1.516	1.095
kag_000_02036	Br ₅ Gd ₃ Ti ₂	10	-3.92	-4.548	-6.000e-06	0.00563	1.636	2.707
kag_000_02044	Co ₄ GeSn ₂ Ta	8	-5.73	-6.404	-1.000e-06	0.00847	0.822	1.761
kag_000_02083	Eu ₃ Na ₂ Yb ₃	8	-1.474	-1.516	-1.000e-06	0.00783	0.683	0.42
kag_000_02098	DySnTb ₃ Yb ₃	8	-3.418	-3.403	0.000e+00	0.00249	0.116	0.115
kag_000_02113	Br ₂ Dy ₄ Fe ₂ LiPtSe ₂	12	-4.44	-5.055	-6.000e-06	0.00558	1.655	2.935
kag_000_02116	Ru ₄ Th ₂	6	-8.904	-8.932	0.000e+00	0.00596	0.13	0.113
kag_000_02149	Dy ₃ Na ₅	8	-2.169	-2.213	-1.000e-06	0.00286	0.27	0.206
kag_000_02152	Nd ₃ SrTl ₃	7	-3.049	-3.499	-1.000e-06	0.00383	1.087	2.097
kag_000_02158	EuGa ₂ Nd ₅	8	-3.923	-4.133	-1.000e-06	0.00645	1.513	2.725
kag_000_02177	Dy ₃ EuInNa ₃	8	-2.623	-2.655	1.000e-06	0.00723	0.338	0.146
kag_000_02182	CeGeHg ₂ Mn ₃ Sb	8	-4.397	-5.223	-1.000e-06	0.00894	1.487	1.913
kag_000_02192	BiEuGd ₄ SnSr	8	-3.737	-4.046	1.000e-06	0.00287	1.727	2.031
kag_000_02206	Al ₅ Mn ₄ Ni ₃	12	-5.965	-6.115	1.000e-06	0.00738	0.611	0.55
kag_000_02217	As ₂ Co ₅ CrSn ₂	10	-5.9	-6.164	-9.200e-05	0.00838	0.44	0.935
kag_000_02225	AlNi ₇	8	-5.351	-5.446	-4.000e-06	0.00879	0.586	1.575
kag_000_02230	Al ₃ Ni ₅	8	-5.056	-5.215	-2.000e-06	0.00375	0.428	0.217
kag_000_02231	Cs ₅ Nd ₃ Sn	9	-1.398	-2.366	-2.700e-05	0.00451	2.417	1.776
kag_000_02236	Na ₅ Tb ₃	8	-2.176	-2.229	5.000e-06	0.00132	0.322	0.383
kag_000_02245	AlMn ₆ Ti	8	-8.079	-8.191	2.000e-06	0.00582	0.672	1.044
kag_000_02265	DyGaPt ₂ Ru ₄	8	-7.092	-7.22	-5.000e-06	0.00458	0.308	0.251
kag_000_02272	Eu ₅ Tb ₃	8	-2.735	-2.741	0.000e+00	0.00148	0.111	0.163
kag_000_02285	CdGd ₇	8	-4.126	-4.146	1.000e-06	0.00179	0.23	0.154
kag_000_02294	Co ₃ Lu ₄ NaPd	9	-4.267	-5.173	2.000e-06	0.00901	1.173	1.797

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_02309	Ga ₅ Tb ₃	8	-3.458	-4.098	1.000e-06	0.00922	1.909	1.935
kag_000_02331	Na ₅ Nd ₃	8	-2.327	-2.329	1.000e-06	0.00474	0.185	1.048
kag_000_02340	Cl ₃ Cs ₂ Gd ₃ Ru	9	-3.572	-4.056	-1.300e-05	0.00497	0.75	2.667
kag_000_02342	CaLa ₂ MgSrTb ₃	8	-3.426	-3.454	3.000e-06	0.00189	0.449	0.311
kag_000_02353	Dy ₃ Rh ₄ S ₅	12	-5.367	-6.314	-5.000e-06	0.00621	1.493	2.973
kag_000_02438	Cs ₂ KNd ₄	7	-2.512	-2.661	-2.000e-06	0.00339	1.308	1.726
kag_000_02440	Ga ₂ Gd ₄ S ₄ Sn	11	-3.826	-5.118	0.000e+00	0.00455	1.916	2.631
kag_000_02446	CaEu ₂ SnSrTb ₃	8	-2.876	-3.171	-4.000e-06	0.00731	1.099	1.215
kag_000_02473	Nd ₃ S ₈ Ti	12	-5.4	-6.07	-2.000e-06	0.00781	1.497	2.119
kag_000_02476	MgMn ₄ Y	6	-6.954	-7.143	1.000e-06	0.0065	0.495	1.131
kag_000_02486	BGePtRu ₄ Tm	8	-6.784	-7.594	0.000e+00	0.0045	1.098	1.891
kag_000_02503	Ga ₄ IrTb ₄	9	-4.34	-4.857	-1.000e-06	0.00833	1.306	1.417
kag_000_02549	CrGd ₃ S ₃ Se ₂ Ti ₂ Zr	12	-5.666	-6.469	-7.000e-06	0.00843	0.647	0.467
kag_000_02565	BaLaNaNd ₄ Sn	8	-3.802	-3.879	0.000e+00	0.00608	1.063	0.587
kag_000_02569	Dy ₄ Ga ₂ IrNbSn ₃ Yb	12	-4.462	-5.107	-5.000e-06	0.00613	1.586	1.059
kag_000_02581	Ca ₂ NaNd ₃ Sn ₂	8	-3.494	-3.71	0.000e+00	0.00312	1.601	2.122
kag_000_02582	NdRbSbTb ₃ TcTl	8	-3.524	-4.024	-2.000e-06	0.00287	1.806	1.996
kag_000_02594	GeNi ₇	8	-5.36	-5.468	1.000e-06	0.00723	0.241	0.141
kag_000_02608	Bi ₂ KYb ₅	8	-2.294	-2.454	1.000e-06	0.00209	1.262	0.848
kag_000_02622	Al ₅ CoRu ₃ TaY ₂	12	-6.594	-6.862	-1.500e-05	0.00753	0.492	1.24
kag_000_02623	FeGa ₂ Mn ₄ Ni	8	-6.697	-6.882	-9.000e-06	0.00726	0.315	1.033
kag_000_02650	ErNaNi ₃ Se ₃	8	-3.762	-4.474	1.700e-05	0.0077	0.84	1.131
kag_000_02655	Dy ₃ Ga ₂ GeMgPdSn ₃	11	-3.903	-4.307	-1.000e-06	0.00418	0.949	1.057
kag_000_02656	Gd ₅ LaSn ₂	8	-4.651	-4.711	-1.000e-06	0.00755	0.338	1.076
kag_000_02663	Nd ₂ Ni ₉	11	-5.471	-5.479	2.000e-06	0.00499	0.125	0.151
kag_000_02682	AsMn ₃ Pt ₃	7	-6.817	-7.032	1.300e-05	0.00897	0.104	1.026
kag_000_02690	Cs ₃ Dy ₃	6	-1.935	-1.958	-8.000e-06	0.00509	0.277	0.334
kag_000_02703	LuTl ₄ Yb ₃	8	-2.155	-2.479	-1.100e-05	0.00635	1.001	0.626
kag_000_02743	Fe ₄ Ge ₂ Sn	7	-6.055	-6.254	1.103e-01	0.00437	0.711	0.453
kag_000_02750	Lu ₂ NaNd ₅	8	-4.095	-4.103	-6.000e-06	0.00383	0.193	0.122
kag_000_02767	GeNi ₆ Rh	8	-5.593	-5.685	1.000e-06	0.00762	0.719	0.92
kag_000_02780	Dy ₃ EuNa ₂ SnTl	8	-3.068	-3.173	-5.000e-06	0.00262	2.033	1.022
kag_000_02785	Ni ₇ Os	8	-5.929	-6.09	-8.000e-06	0.00522	0.696	0.312
kag_000_02801	CaCl ₅ Rh ₂ Yb ₃	11	-3.087	-4.201	-2.600e-05	0.00378	1.73	4.452
kag_000_02804	Dy ₄ GeLu ₂ Sn	8	-4.568	-4.641	-2.000e-06	0.00476	0.353	0.148
kag_000_02806	GeMgNi ₅ Zn	8	-4.354	-4.435	-2.000e-06	0.00491	0.355	0.24
kag_000_02808	Br ₂ CaTb ₃ Tl ₂	8	-2.966	-3.666	0.000e+00	0.00322	1.443	3.072
kag_000_02809	Cl ₅ Mn ₂ Tb ₃	10	-4.312	-5.121	-4.000e-06	0.00784	1.424	4.23
kag_000_02826	Al ₂ GeMn ₄	7	-6.485	-6.74	0.000e+00	0.00652	0.352	1.705
kag_000_02829	Ba ₃ CaEuNd ₃	8	-2.601	-2.785	-1.400e-05	0.00381	0.45	0.605
kag_000_02836	BaSn ₃ Yb ₃	7	-2.431	-3.047	1.000e-06	0.00448	1.906	2.357
kag_000_02859	Ni ₄ Pt ₄	8	-5.309	-5.811	-1.000e-06	0.00497	0.863	0.461
kag_000_02861	Dy ₃ Na ₅	8	-2.174	-2.216	-4.000e-06	0.00309	0.375	1.095
kag_000_02869	Al ₃ Ni ₈	11	-5.177	-5.299	-5.000e-06	0.0097	1.164	0.862
kag_000_02887	NiPt ₃ Ru ₄	8	-7.444	-7.505	-1.300e-05	0.00518	0.146	0.795
kag_000_02985	LaNd ₃ Tl ₄	8	-3.703	-3.77	-3.000e-06	0.00667	0.45	0.264
kag_000_02996	AlGaNi ₂ RhRu ₃	8	-6.67	-6.694	-1.000e-06	0.0062	0.187	0.168
kag_000_02997	Al ₃ Co ₅	8	-5.914	-6.158	1.000e-06	0.00457	0.668	0.977
kag_000_03054	Ba ₂ Dy ₃ EuTl ₂	8	-2.867	-3.028	-3.000e-06	0.00515	1.822	2.06
kag_000_03086	Ru ₄ Tb ₂	6	-7.84	-7.945	-2.000e-06	0.00399	0.24	0.109
kag_000_03095	Fe ₆ OsTi	8	-8.444	-8.47	-2.000e-06	0.00342	0.156	0.126
kag_000_03102	Gd ₃ Na ₅	8	-2.238	-2.248	-3.000e-06	0.00256	0.224	0.97

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_03116	MnNi ₄ P ₃	8	-5.699	-6.217	-1.000e-06	0.00875	0.838	1.25
kag_000_03126	CoFe ₂ Ge ₂ Ni ₃	8	-6.009	-6.097	-3.000e-06	0.00947	0.373	0.205
kag_000_03139	BrINd ₃ RhSnTl	8	-3.951	-4.507	-1.000e-06	0.00569	1.097	1.66
kag_000_03164	GaMn ₄ Pt ₃	8	-7.046	-7.192	1.000e-06	0.00608	0.321	2.138
kag_000_03184	Co ₄ Ho ₂	6	-6.214	-6.397	0.000e+00	0.00628	0.331	1.086
kag_000_03202	GaLaPt ₃ Ru ₃	8	-6.625	-6.767	-4.000e-06	0.00416	0.216	0.195
kag_000_03205	LaMn ₃ Sn ₂ Zn	7	-4.568	-5.783	-6.000e-06	0.00444	1.09	1.754
kag_000_03208	CaEuNa ₂ Yb ₄	8	-1.439	-1.475	-3.000e-06	0.00556	0.742	0.452
kag_000_03218	BiEuNa ₃ Tb ₃	8	-2.85	-2.925	0.000e+00	0.00807	0.669	1.326
kag_000_03251	Co ₃ FeNi ₄	8	-6.132	-6.214	-1.100e-05	0.00429	0.362	0.219
kag_000_03287	Fe ₃ Ni ₅	8	-6.27	-6.313	-2.000e-06	0.007	0.249	0.221
kag_000_03309	Br ₃ Gd ₃ IrKSn	9	-3.772	-4.624	-2.000e-06	0.0051	2.268	2.778
kag_000_03341	Nd ₃ Te ₂ Tl ₂	7	-3.936	-4.088	2.000e-06	0.00263	0.493	0.348
kag_000_03342	Al ₂ Cd ₃ Fe ₃ Tm ₄	12	-4.318	-4.548	2.000e-06	0.00565	0.4	0.455
kag_000_03358	CoFe ₆ Si ₂ Zr ₃	12	-7.671	-8.073	3.000e-06	0.00445	0.376	1.027
kag_000_03359	Dy ₃ Na ₂ Tl ₃	8	-2.725	-2.96	-7.000e-06	0.00473	0.926	2.228
kag_000_03408	Dy ₄ Na ₄	8	-2.566	-2.599	2.000e-06	0.0046	0.573	0.383
kag_000_03418	EuIn ₃ PbTb ₃	8	-3.489	-3.716	-3.000e-06	0.00618	0.575	0.373
kag_000_03431	Al ₃ CrDy ₃ S ₅	12	-4.645	-5.486	-5.400e-05	0.00493	1.411	3.407
kag_000_03439	Dy ₃ Pd ₄ Se ₅	12	-4.709	-5.34	-2.000e-06	0.0047	2.267	2.483
kag_000_03453	Dy ₃ Na ₅	8	-2.152	-2.22	2.000e-06	0.00634	0.544	0.277
kag_000_03463	FeNi ₄ Zr ₄	9	-7.089	-7.302	-3.000e-06	0.00551	0.378	0.906
kag_000_03495	Co ₄ Fe ₃ Ni	8	-6.857	-7.093	-2.000e-06	0.00589	0.284	0.231
kag_000_03512	Eu ₂ In ₃ Yb ₃	8	-2.006	-2.226	-3.000e-06	0.00183	0.998	0.499
kag_000_03522	AlAuGeMn ₃ Tb	7	-5.837	-6.182	0.000e+00	0.00573	0.729	0.764
kag_000_03539	Dy ₂ Mn ₄	6	-7.346	-7.367	-4.000e-06	0.00386	0.098	0.05
kag_000_03543	AsLaNa ₃ Ru ₃	8	-4.259	-4.823	-1.300e-05	0.00655	1.274	1.479
kag_000_03564	Dy ₄ EuInLaPt	8	-4.248	-4.558	-1.000e-06	0.00599	1.174	2.955
kag_000_03577	AlPt ₄ Ru ₃	8	-6.968	-7.137	-1.000e-06	0.00474	0.336	0.917
kag_000_03592	Nd ₄ SnTl ₃	8	-3.658	-3.995	-6.000e-06	0.0069	0.815	1.446
kag_000_03594	FeNi ₁₀	11	-5.478	-5.505	-1.100e-05	0.00988	0.112	0.13
kag_000_03629	Ga ₃ Ni ₅	8	-4.727	-4.84	3.000e-06	0.00744	0.764	0.938
kag_000_03636	Cl ₃ CoCsGd ₃	8	-3.647	-4.392	-2.100e-05	0.00479	2.151	3.357
kag_000_03637	AcDy ₄ EuNaSr	8	-3.001	-3.191	-3.000e-05	0.00452	0.572	0.625
kag_000_03651	CaGd ₃ MgPbSr	7	-3.038	-3.272	-9.000e-06	0.00316	1.2	2.625
kag_000_03670	Co ₄ GdPt ₂	7	-6.083	-6.531	0.000e+00	0.00758	0.721	0.683
kag_000_03681	AsAu ₂ Br ₃ Ru ₃	9	-3.974	-4.515	-3.000e-06	0.00705	0.554	2.522
kag_000_03699	Ag ₂ NaNi ₃ Sn	7	-3.504	-3.703	-1.000e-06	0.00367	0.547	0.356
kag_000_03724	Pt ₄ Ru ₃ Zn	8	-6.61	-6.682	1.000e-06	0.0078	0.216	0.259
kag_000_03725	Hf ₂ Ru ₄ Sn	7	-8.57	-8.757	-2.000e-06	0.00345	0.27	0.529
kag_000_03728	S ₅ Tb ₃ W ₄	12	-6.653	-7.611	-2.000e-06	0.0035	0.683	2.732
kag_000_03732	B ₂ Ru ₃ S ₅ Sr	11	-5.603	-6.049	-1.000e-06	0.00875	0.508	1.127
kag_000_03746	Gd ₃ Sr ₂ Tl ₃	8	-2.885	-3.1	0.000e+00	0.00298	1.253	3.411
kag_000_03752	BaCaGd ₃ SbSmSr	8	-3.529	-3.536	-4.000e-06	0.00204	0.205	0.16
kag_000_03756	Eu ₂ Gd ₄ Ge ₂	8	-3.872	-4.229	-2.000e-06	0.00963	1.013	0.833
kag_000_03772	CaCdDyMg ₃ Ru ₃ Si	10	-4.209	-4.609	-4.000e-06	0.00456	1.209	1.377
kag_000_03808	Bi ₃ Dy ₃ Tl ₂	8	-4.019	-4.062	0.000e+00	0.00326	0.212	0.378
kag_000_03817	Co ₈	8	-6.659	-6.84	-1.000e-06	0.00936	0.448	0.296
kag_000_03845	Al ₂ Co ₃ Fe ₃ Hf ₄	12	-8.136	-8.164	-4.000e-06	0.00661	0.118	0.113
kag_000_03847	Dy ₃ EuGaLuTl	7	-3.252	-3.76	-8.000e-06	0.0081	2.184	1.948
kag_000_03852	Br ₃ Tb ₃	6	-3.143	-4.182	-1.000e-06	0.00233	1.605	2.694
kag_000_03870	Ni ₃ ScSiSn ₂	7	-5.146	-5.362	-3.000e-06	0.00566	0.367	1.777

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_03889	Dy ₃ Na ₃ SbTl	8	-3.011	-3.176	2.000e-06	0.00629	0.464	0.578
kag_000_03890	Eu ₂ Na ₂ RbYb ₃	8	-1.288	-1.332	-1.000e-06	0.00276	0.394	0.382
kag_000_03909	Ge ₂ LuRu ₃ SbSiZr ₄	12	-7.32	-7.55	0.000e+00	0.00558	0.497	0.558
kag_000_03913	AlNi ₄ Pt ₃	8	-5.635	-5.811	-5.900e-05	0.00623	0.335	0.161
kag_000_03954	Fe ₇ Pt	8	-7.306	-7.798	0.000e+00	0.0059	0.729	0.477
kag_000_03956	Dy ₃ S ₅ V ₄	12	-5.876	-6.736	-9.000e-06	0.00976	0.948	2.721
kag_000_03971	EuLuTb ₃ Tl ₃	8	-3.149	-3.557	0.000e+00	0.00787	1.683	1.636
kag_000_03999	FeGa ₂ Ni ₃ Si	7	-5.021	-5.266	-1.000e-06	0.0055	0.353	0.56
kag_000_04001	AlNi ₇	8	-5.411	-5.444	3.000e-06	0.00649	0.279	0.755
kag_000_04018	Fe ₃ GaLaSn ₂ Zn	8	-4.292	-5.131	-1.100e-05	0.00643	1.24	1.611
kag_000_04037	Co ₄ LiNa	6	-4.372	-4.732	-5.000e-06	0.00654	0.81	2.636
kag_000_04046	Eu ₅ Yb ₃	8	-1.55	-1.708	-1.000e-06	0.00235	1.116	2.065
kag_000_04052	Co ₆ GePt	8	-6.5	-6.524	-1.000e-06	0.00647	0.127	0.16
kag_000_04090	CuFe ₃ Ga ₄	8	-4.795	-4.917	1.000e-06	0.00728	0.88	0.846
kag_000_04113	Co ₃ LiSSn ₃	8	-4.218	-4.807	0.000e+00	0.00719	1.733	1.052
kag_000_04124	Al ₃ GaMn ₃ Ru	8	-6.225	-6.394	-2.000e-06	0.00385	0.699	1.032
kag_000_04159	Eu ₃ Yb ₅	8	-1.55	-1.606	0.000e+00	0.00223	1.237	0.574
kag_000_04160	Cs ₄ Dy ₃	7	-1.841	-1.853	-2.000e-06	0.00156	0.234	0.256
kag_000_04179	Cs ₄ Gd ₃	7	-1.884	-1.896	-3.000e-06	0.00181	0.229	0.252
kag_000_04185	Nd ₃ Sb ₂ TeTl	7	-4.201	-4.761	-2.000e-06	0.00329	1.73	1.449
kag_000_04224	Na ₅ Yb ₃	8	-1.262	-1.287	2.000e-06	0.00412	0.136	1.206
kag_000_04255	CePt ₃ RhRu ₃	8	-7.321	-7.627	-2.000e-06	0.00763	0.474	1.931
kag_000_04307	Al ₂ Fe ₃ Hf ₂ Nb ₃ Zr	11	-8.175	-8.328	-4.000e-06	0.00765	0.225	0.356
kag_000_04354	FeGaNi ₄ SnTi	8	-5.385	-5.627	-2.000e-06	0.00644	0.489	0.368
kag_000_04359	BaCeNd ₃ Sb ₂ Sn	8	-4.366	-4.825	-2.500e-05	0.00578	2.0	2.109
kag_000_04373	MgRu ₄ Y ₂	7	-6.919	-7.383	1.000e-06	0.00356	0.352	1.146
kag_000_04390	BrSnTb ₃ Tl ₂	7	-3.043	-3.904	-9.000e-06	0.00682	1.848	3.162
kag_000_04419	Co ₃ Pt ₅	8	-6.189	-6.329	-1.800e-05	0.00533	0.513	1.595
kag_000_04421	AlMn ₃ Sn ₂	6	-5.568	-6.117	-3.000e-06	0.00694	0.878	1.54
kag_000_04441	Co ₃ Dy ₂ Mn	6	-6.571	-6.629	-8.000e-06	0.00899	0.237	0.221
kag_000_04461	Co ₈	8	-6.653	-6.839	0.000e+00	0.00698	0.508	0.919
kag_000_04476	Mn ₈	8	-8.818	-8.922	2.000e-06	0.00174	0.268	0.16
kag_000_04512	Ga ₂ Lu ₄ Ni ₃ W	10	-5.329	-5.521	0.000e+00	0.00871	0.807	0.8
kag_000_04519	Co ₄ Pt ₄	8	-5.984	-6.434	-2.400e-05	0.0094	0.349	0.873
kag_000_04541	LuPb ₂ Tb ₅	8	-4.361	-4.585	0.000e+00	0.007	0.66	0.306
kag_000_04542	PrRu ₄ Y	6	-7.929	-8.194	-1.000e-06	0.00649	0.323	0.229
kag_000_04543	IrNdPtRu ₃ Sn	7	-6.82	-7.435	-1.000e-06	0.00626	0.462	1.838
kag_000_04578	Co ₂ Nd ₃ Se ₅ Ti ₂	12	-5.211	-5.939	-1.100e-05	0.00677	1.002	2.108
kag_000_04596	Br ₅ RhTb ₃	9	-3.885	-4.51	-9.000e-06	0.00644	0.972	2.684
kag_000_04597	Al ₂ Pt ₂ Ru ₄	8	-7.074	-7.34	-6.000e-06	0.00302	0.389	0.292
kag_000_04610	Co ₃ Pt ₃ Y ₄	10	-7.147	-7.188	-1.700e-05	0.00759	0.27	0.315
kag_000_04631	Br ₃ RbSnTb ₃	8	-2.893	-3.843	-1.000e-06	0.0039	1.642	3.103
kag_000_04636	Cl ₅ MnTeYb ₃	10	-2.887	-3.996	8.000e-06	0.00396	2.413	2.74
kag_000_04650	BaCeGa ₂ Nd ₃ Tl	8	-3.733	-3.948	1.000e-06	0.00204	1.255	3.387
kag_000_04676	Mn ₄ PtRuSi ₂	8	-7.773	-7.953	-1.100e-05	0.00539	0.424	0.391
kag_000_04684	AuCo ₃ Sn ₃	7	-4.752	-5.08	-2.000e-06	0.00915	0.902	1.248
kag_000_04720	Co ₂ GeNi ₄ Pd	8	-5.677	-5.696	-7.000e-06	0.00953	0.061	0.044
kag_000_04723	Fe ₅ Pt ₃	8	-7.277	-7.293	-5.400e-05	0.00668	0.081	0.692
kag_000_04774	Bi ₄ Dy ₃ Eu	8	-4.016	-4.414	0.000e+00	0.00551	0.766	2.422
kag_000_04787	Nd ₄ Sn ₂ Te ₂	8	-4.57	-4.791	0.000e+00	0.00232	0.878	2.091
kag_000_04797	Co ₃ DyLiSe ₃	8	-4.632	-5.146	2.000e-06	0.00828	1.308	1.245
kag_000_04807	Ga ₂ Ni ₃ Tb ₂	7	-4.812	-4.838	-1.000e-05	0.00865	0.146	0.125

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_04819	Al ₃ Fe ₃ Nb ₄ Si ₂	12	-7.394	-7.636	-2.000e-06	0.00354	0.475	0.522
kag_000_04835	H ₃ GeMn ₃ Pt	8	-4.956	-5.898	2.000e-06	0.00769	0.837	2.342
kag_000_04854	CuFe ₆ Ni ₄ Rh	12	-6.552	-6.643	-2.000e-06	0.00494	0.199	0.227
kag_000_04857	FeGaGeNi ₅	8	-5.334	-5.542	-8.000e-06	0.00611	0.757	0.677
kag_000_04875	H ₃ Fe ₃ IrNi ₂	9	-4.932	-5.86	-3.000e-05	0.0084	0.523	0.825
kag_000_04876	Ga ₄ LiMn ₃	8	-4.665	-4.95	-1.000e-06	0.00291	0.594	1.744
kag_000_04897	BaGeK ₂ LaNa ₃ SnYb ₃	12	-1.984	-2.225	-1.000e-06	0.00841	1.894	2.098
kag_000_04899	AlMn ₃ Sn ₃	7	-5.213	-5.744	-1.000e-06	0.00738	0.742	0.753
kag_000_04909	Na ₄ Ni ₃	7	-2.636	-2.733	0.000e+00	0.00475	0.571	0.547
kag_000_04918	Al ₂ Ga ₆ NiRu ₃	12	-4.808	-5.019	-1.000e-06	0.00884	0.573	1.009
kag_000_04925	Co ₆ Pt ₂	8	-6.566	-6.62	0.000e+00	0.00927	0.178	0.197
kag_000_04953	CoNi ₅ PtSi	8	-5.787	-5.905	-2.000e-05	0.00978	0.431	0.226
kag_000_04957	BaI ₃ RhSnTb ₃	9	-3.536	-4.258	-1.800e-05	0.00352	1.51	3.398
kag_000_04980	LiNi ₃ Sn ₄	8	-3.558	-4.305	-1.100e-05	0.00735	1.091	1.283
kag_000_04997	Ag ₂ Ge ₂ PdSnTb ₃	9	-4.185	-4.557	-4.000e-06	0.00206	0.807	1.503
kag_000_05004	Ba ₂ CaCdSnYb ₃	8	-1.907	-2.06	-9.000e-06	0.00374	2.281	2.415
kag_000_05017	CsDy ₃ S ₅	9	-5.406	-5.673	-4.000e-06	0.00482	1.115	1.17
kag_000_05019	As ₄ CuFe ₃ Na ₂	10	-4.838	-5.015	0.000e+00	0.0096	0.769	1.407
kag_000_05024	Bi ₄ NaTb ₃	8	-4.131	-4.194	-1.200e-05	0.00351	0.85	2.186
kag_000_05048	Co ₅ Fe ₂ Ni	8	-6.674	-6.937	-4.000e-06	0.00784	0.695	1.096
kag_000_05056	Ga ₃ Ni ₅	8	-4.716	-4.838	0.000e+00	0.00422	0.464	0.99
kag_000_05073	GaMn ₃ SnZnZr	7	-6.055	-6.133	1.000e-06	0.00392	0.179	0.175
kag_000_05087	AuCa ₂ Ru ₃	6	-5.618	-5.883	0.000e+00	0.00198	0.385	0.229
kag_000_05100	Dy ₃ RhTl ₅	9	-3.667	-3.819	-3.000e-06	0.00378	0.918	1.064
kag_000_05105	InPbTl ₂ Yb ₃	7	-2.257	-2.472	-5.000e-06	0.00568	1.978	1.39
kag_000_05111	Al ₂ Mn ₄ Sn	7	-6.169	-6.568	-2.000e-06	0.00721	0.701	0.655
kag_000_05122	Cl ₃ Cs ₂ Gd ₃ Pt	9	-3.415	-3.943	-2.000e-06	0.00521	0.937	3.283
kag_000_05194	Eu ₂ InYb ₅	8	-1.752	-1.769	-3.000e-06	0.00313	0.277	0.179
kag_000_05208	Al ₄ Ru ₄	8	-6.488	-6.901	-4.000e-06	0.00478	0.673	2.005
kag_000_05213	Ce ₂ Dy ₄ Na ₂	8	-3.751	-3.788	-2.400e-05	0.00969	0.413	1.968
kag_000_05241	AlGaMgNd ₄ Sn	8	-3.963	-4.132	-1.200e-05	0.00555	0.659	0.325
kag_000_05266	Ge ₂ Pd ₄ Yb ₆	12	-3.659	-3.926	-4.000e-06	0.00303	1.16	1.583
kag_000_05271	EuNa ₄ Yb ₃	8	-1.311	-1.352	3.000e-06	0.00366	1.147	1.568
kag_000_05307	Gd ₃ I ₅ Pd ₂	10	-3.347	-4.101	-7.000e-06	0.00503	2.705	3.617
kag_000_05311	Fe ₃ Ga ₄	7	-4.905	-5.077	4.000e-06	0.00832	0.258	0.209
kag_000_05327	GaNi ₅ Sn ₂	8	-4.73	-4.868	0.000e+00	0.00988	0.433	0.278
kag_000_05405	CaEuPtRu ₃ Y	7	-5.924	-6.46	-1.100e-05	0.00773	0.614	1.535
kag_000_05409	Na ₃ Yb ₅	8	-1.325	-1.329	1.000e-06	0.00233	0.561	1.215
kag_000_05418	AlNi ₇	8	-5.389	-5.446	-1.000e-06	0.0056	0.364	0.192
kag_000_05421	Ge ₂ LaOs ₂ PdRu ₃ SbSr	11	-6.347	-6.726	-4.000e-06	0.00336	0.572	0.646
kag_000_05463	CaNa ₄ Tb ₃	8	-2.319	-2.329	-2.000e-06	0.00342	0.975	0.541
kag_000_05466	Dy ₃ K ₂ NaSb ₂	8	-3.189	-3.389	1.000e-06	0.00432	0.715	1.722
kag_000_05477	EuNa ₃ Nd ₃ Pb	8	-2.877	-2.923	3.000e-06	0.00773	0.619	0.355
kag_000_05494	Al ₃ Ni ₅	8	-5.279	-5.351	-1.900e-05	0.00583	0.457	0.368
kag_000_05537	Ga ₄ Ni ₄ Tm ₄	12	-4.474	-4.837	-2.000e-06	0.00773	0.635	0.543
kag_000_05553	Co ₂ Ni ₅ Re	8	-6.58	-6.63	3.000e-06	0.00942	0.169	0.166
kag_000_05586	CoNi ₇	8	-5.452	-5.568	1.500e-05	0.0041	0.705	0.951
kag_000_05642	Al ₂ Co ₃ Er ₄ Ni ₃	12	-5.563	-5.711	-2.000e-06	0.00592	0.307	0.239
kag_000_05650	Cl ₄ CsDy ₃ N	9	-3.561	-4.817	0.000e+00	0.00727	1.978	2.311
kag_000_05654	EuInTb ₄ Tl ₂	8	-3.456	-3.663	-1.400e-05	0.00744	0.74	0.502
kag_000_05673	Br ₃ ClDy ₃ MnRb	9	-3.657	-4.026	-1.000e-06	0.00547	1.211	1.125
kag_000_05682	Ga ₄ Ru ₃ Y	8	-5.589	-5.984	1.000e-06	0.00732	0.821	2.252

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_05692	Br ₂ Gd ₄ PbPt	8	-4.203	-4.873	0.000e+00	0.00701	1.377	3.23
kag_000_05706	Nd ₃ Sn ₃ SrYb	8	-3.984	-4.046	0.000e+00	0.00594	0.356	0.24
kag_000_05734	BrGd ₃ PrTe ₆ Tl	12	-4.125	-4.71	-2.800e-05	0.00388	1.155	2.188
kag_000_05772	Dy ₃ Na ₅	8	-2.182	-2.213	-3.000e-06	0.00112	0.383	1.193
kag_000_05790	Cu ₂ Ga ₂ Ni ₆ PSi	12	-4.844	-4.998	-2.000e-06	0.00803	0.397	0.537
kag_000_05793	GaMn ₃ S ₂ Sn ₃ Tb ₃	12	-5.049	-5.568	-5.000e-06	0.00573	0.806	3.976
kag_000_05798	AlGa ₂ Ni ₅	8	-4.891	-5.009	1.000e-06	0.00793	0.494	0.887
kag_000_05826	Fe ₄ PdPt ₃	8	-6.68	-6.856	-2.200e-05	0.00691	0.397	0.82
kag_000_05836	Dy ₃ GeInLuSr ₂	8	-3.486	-3.658	0.000e+00	0.00715	1.718	1.126
kag_000_05861	EuIr ₂ Na ₄ Yb ₃	10	-2.595	-2.947	-2.000e-06	0.00624	0.732	1.424
kag_000_05908	K ₅ Yb ₃	8	-0.953	-1.041	-5.000e-06	0.00446	1.43	1.724
kag_000_05923	Dy ₃ Ga ₂ PrSn	7	-3.992	-4.473	-3.000e-06	0.00784	1.552	3.178
kag_000_05947	Cs ₄ Yb ₃	7	-0.91	-0.93	-1.490e-05	0.00107	0.424	0.337
kag_000_05951	AlCoMn ₃ NiRuU	8	-7.698	-8.055	-1.000e-06	0.0068	1.021	1.512
kag_000_05981	Gd ₃ Na ₉	12	-1.938	-1.942	0.000e+00	0.00553	0.143	0.183
kag_000_05991	As ₂ GdGe ₃ Ru ₃ Te	10	-5.753	-6.107	-1.000e-06	0.00609	0.506	1.224
kag_000_05995	Co ₇ Y	8	-6.564	-6.634	-2.000e-06	0.00771	0.249	0.244
kag_000_06002	AgEuTl ₂ Yb ₃	7	-1.82	-2.282	-1.000e-06	0.00624	2.121	1.947
kag_000_06026	Bi ₂ Tl ₃ Yb ₃	8	-2.258	-2.764	0.000e+00	0.00377	1.089	0.737
kag_000_06113	Pd ₄ Ru ₃ Sn	8	-6.322	-6.477	-3.000e-06	0.00388	0.471	0.988
kag_000_06148	Co ₄ Tm ₂	6	-6.313	-6.418	3.000e-06	0.00923	0.188	0.17
kag_000_06151	Mn ₄ Se ₄	8	-5.734	-6.458	0.000e+00	0.00776	1.035	0.795
kag_000_06162	AgMnRu ₃ S ₃ Sn ₄	12	-4.948	-5.592	-6.000e-06	0.00913	0.684	1.628
kag_000_06183	AlGaNi ₃ SnTb	7	-4.7	-4.81	0.000e+00	0.00471	0.489	0.595
kag_000_06188	BrCl ₃ Dy ₃ IrRb	9	-3.757	-4.604	-6.000e-06	0.00524	1.63	2.346
kag_000_06190	Al ₂ BDy ₂ Ru ₇	12	-7.271	-7.484	-3.000e-05	0.00921	0.631	0.633
kag_000_06198	EuMn ₃ Sn ₃ Te	8	-4.72	-5.578	1.000e-06	0.00611	1.249	1.624
kag_000_06199	DyLuNi ₄	6	-5.504	-5.631	-4.000e-06	0.00689	0.317	0.123
kag_000_06241	NbNi ₇	8	-6.007	-6.145	-1.000e-05	0.00865	0.362	0.304
kag_000_06253	Dy ₃ GaIr ₄ NdSn ₂	11	-6.042	-6.34	2.000e-06	0.00623	0.682	1.29
kag_000_06264	Co ₃ Ga ₂ Mn ₃ Zr ₄	12	-7.637	-7.698	-3.000e-06	0.00536	0.187	0.135
kag_000_06273	CoFe ₂ Ni ₅	8	-5.999	-6.182	-1.900e-05	0.00651	0.349	0.221
kag_000_06282	FeNi ₆ Rh	8	-5.895	-5.924	-6.000e-06	0.0052	0.219	0.197
kag_000_06285	AlCoCrMn ₃ PtSi	8	-7.355	-7.501	0.000e+00	0.00522	0.685	1.293
kag_000_06291	Dy ₈	8	-4.377	-4.524	0.000e+00	0.00309	0.228	1.294
kag_000_06304	CrDy ₃ GeLa ₂ STe ₂ Zn	11	-4.748	-5.143	-6.000e-06	0.00935	1.658	3.284
kag_000_06325	CaCeSnTb ₃ Tl ₂	8	-3.952	-4.014	0.000e+00	0.00407	0.429	0.275
kag_000_06346	Co ₈	8	-6.715	-6.84	2.000e-06	0.00787	0.219	0.166
kag_000_06364	Co ₂ Fe ₃ MgNi ₅ V	12	-6.15	-6.242	-8.300e-05	0.00346	0.296	0.213
kag_000_06396	Ge ₂ Pt ₂ Ru ₄	8	-6.968	-7.322	-1.000e-06	0.00698	0.48	1.725
kag_000_06401	S ₈ TaTb ₃	12	-6.119	-6.237	-2.000e-06	0.00812	0.67	1.757
kag_000_06432	Co ₃ Ni ₅	8	-5.746	-5.9	-6.000e-06	0.00405	0.357	0.275
kag_000_06434	Al ₂ EuLu ₂ Nd ₃ Ni ₃	11	-4.406	-4.709	-8.000e-06	0.00691	0.472	1.231
kag_000_06440	Lu ₄ Nd ₃ Pb	8	-4.394	-4.485	0.000e+00	0.00572	0.412	0.339
kag_000_06443	Nd ₄ Tl ₄	8	-3.6	-3.76	0.000e+00	0.00296	0.384	1.449
kag_000_06455	AlFe ₃ Y ₂	6	-6.927	-6.952	-6.000e-06	0.00571	0.064	1.006
kag_000_06458	CaCo ₄ Er	6	-5.677	-5.767	1.000e-06	0.00415	0.381	0.233
kag_000_06516	Co ₄ Er ₂	6	-6.299	-6.409	-2.000e-06	0.00981	0.215	0.178
kag_000_06524	Ru ₄ Si ₂ UZn	8	-7.428	-7.747	1.000e-06	0.00532	0.565	0.46
kag_000_06527	Br ₅ Ru ₂ Tb ₃	10	-4.076	-4.856	-5.500e-05	0.00636	1.995	2.529
kag_000_06532	AsNi ₄ PSeU	8	-5.669	-6.168	1.000e-06	0.00713	1.076	1.901
kag_000_06539	Co ₃ PtRu ₃ U	8	-8.264	-8.317	0.000e+00	0.00614	0.239	0.807

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_06621	AlFe ₄ ScSi ₂ Ti ₂	10	-7.028	-7.279	-5.000e-06	0.00516	0.562	0.398
kag_000_06625	AsGePRu ₅	8	-6.978	-7.581	-4.000e-06	0.00627	0.423	1.649
kag_000_06635	Ga ₄ Gd ₄	8	-3.817	-4.207	-3.000e-06	0.00535	1.103	2.619
kag_000_06647	Dy ₃ EuGeLuSnYb	8	-3.803	-4.058	-1.000e-06	0.00681	0.811	0.654
kag_000_06697	Ge ₈ Mn ₃ Yb	12	-4.938	-5.338	-6.000e-06	0.00597	0.968	2.215
kag_000_06741	Na ₅ Yb ₃	8	-1.269	-1.283	-2.600e-05	0.0036	0.439	0.21
kag_000_06758	AlCo ₂ Fe ₉	12	-7.403	-7.561	-4.000e-06	0.00402	0.256	0.226
kag_000_06764	Cs ₄ Dy ₃	7	-1.845	-1.855	1.000e-06	0.00177	0.154	0.215
kag_000_06770	HGaNi ₆ SnTl ₃	12	-3.831	-3.996	0.0000e+00	0.00863	0.514	2.676
kag_000_06787	Eu ₃ GeInTb ₃	8	-3.301	-3.577	0.0000e+00	0.00802	1.804	2.499
kag_000_06788	Ni ₃ SbScSe ₂	7	-4.859	-5.333	0.0000e+00	0.00862	0.558	0.739
kag_000_06794	Co ₅ Fe ₃	8	-7.228	-7.304	-2.700e-05	0.00708	0.211	0.163
kag_000_06802	Pt ₄ RhRu ₃	8	-7.278	-7.348	-3.000e-06	0.00465	0.196	0.178
kag_000_06817	La ₃ Ni ₄ Si ₂	9	-5.63	-5.755	0.0000e+00	0.00884	0.35	0.429
kag_000_06818	Co ₃ DyLiSe ₂ Y	8	-4.255	-5.525	-2.000e-06	0.00615	1.921	0.891
kag_000_06822	Cl ₄ CsIrNd ₃	9	-3.764	-4.779	-1.500e-05	0.00652	0.761	2.121
kag_000_06829	InNa ₂ Tb ₄ Tl	8	-3.329	-3.202	-1.000e-06	0.005	0.704	2.958
kag_000_06841	BrCl ₂ CsGd ₃ Ir	8	-3.73	-4.635	0.0000e+00	0.00663	1.988	3.914
kag_000_06844	AlFe ₅ Ga ₂	8	-6.097	-6.312	-4.000e-06	0.00358	0.245	1.672
kag_000_06879	Dy ₃ SrTl ₄	8	-3.083	-3.223	-1.000e-06	0.00605	0.323	1.29
kag_000_06893	Cs ₄ Dy ₃	7	-1.838	-1.853	-2.000e-06	0.00305	0.21	0.223
kag_000_06907	Ga ₄ Ni ₄	8	-4.316	-4.408	0.0000e+00	0.0038	0.579	0.295
kag_000_06921	LaTl ₃ Yb ₃	7	-2.202	-2.672	-1.400e-05	0.00307	1.29	2.981
kag_000_06927	Ca ₂ Tb ₃ Tl ₃	8	-2.777	-3.253	-4.000e-06	0.00452	1.011	1.442
kag_000_06934	PtRh ₄ Ru ₃	8	-7.417	-7.795	-8.000e-06	0.00684	0.726	0.446
kag_000_06959	Al ₄ Co ₃ LaSi	9	-5.47	-5.541	-4.000e-06	0.00915	0.299	0.299
kag_000_06976	MnSe ₈ Tb ₃	12	-4.896	-5.21	0.0000e+00	0.00425	1.112	2.647
kag_000_06987	Na ₅ Tb ₃	8	-2.188	-2.234	-5.000e-06	0.00583	0.948	1.552
kag_000_07005	CeNa ₂ Nd ₃ Sn ₂	8	-3.852	-4.041	2.000e-06	0.00804	1.407	4.154
kag_000_07013	Cs ₄ Dy ₃	7	-1.84	-1.853	0.0000e+00	0.00333	0.264	0.297
kag_000_07028	As ₂ Br ₃ ClITb ₃	10	-3.233	-4.562	-1.000e-06	0.00279	1.93	4.409
kag_000_07038	Br ₃ CrNaNiSnTb ₃	10	-3.855	-4.22	-9.000e-06	0.00673	2.117	1.956
kag_000_07071	Co ₄ Mn ₄	8	-7.668	-7.937	-6.000e-06	0.00917	0.456	0.895
kag_000_07072	GaNbTb ₃ Tl ₃	8	-3.178	-3.257	0.0000e+00	0.0046	0.769	0.743
kag_000_07073	Dy ₃ Ga ₄ Lu	8	-3.775	-4.156	0.0000e+00	0.00532	1.084	2.512
kag_000_07096	Br ₅ GaNd ₃ Ru ₂	11	-4.034	-4.847	-1.700e-05	0.00782	1.927	3.751
kag_000_07099	AlMn ₃ Pt ₄	8	-6.789	-7.081	1.000e-06	0.00608	0.062	1.5
kag_000_07101	EuLuNaTiYb ₄	8	-1.86	-1.949	-2.000e-06	0.00912	1.026	0.506
kag_000_07132	Dy ₃ EuInNa ₂ Tl	8	-2.722	-2.973	-2.000e-06	0.00566	1.63	1.871
kag_000_07133	AlCo ₃ Ge ₂ Nd ₂	8	-5.098	-5.663	1.000e-06	0.00413	1.389	1.346
kag_000_07158	Eu ₃ Ga ₂ Nd ₃	8	-3.207	-3.431	0.0000e+00	0.00387	1.666	1.852
kag_000_07178	BrCl ₇ Gd ₃ Na	12	-4.276	-4.437	-1.000e-06	0.00519	0.816	1.581
kag_000_07183	Fe ₃ GaIrMgPt	7	-6.018	-6.277	-1.000e-06	0.00548	0.323	1.096
kag_000_07216	CaNa ₄ Yb ₃	8	-1.318	-1.351	-1.000e-06	0.00316	0.539	0.407
kag_000_07221	Co ₆ GaPt	8	-6.311	-6.334	-8.000e-06	0.00909	0.128	0.753
kag_000_07248	AlCo ₄ FeGa ₂	8	-5.783	-5.899	-3.800e-05	0.00732	0.454	0.441
kag_000_07298	Cl ₃ CsIIrYb ₃	9	-2.863	-3.544	-1.400e-05	0.00716	1.78	2.241
kag_000_07307	Co ₄ Ga ₄ Sr	9	-4.589	-4.629	-2.000e-06	0.00795	0.434	0.999
kag_000_07333	BaGaGd ₄ KPt	8	-3.592	-3.916	-4.000e-06	0.00531	1.503	2.036
kag_000_07339	Lu ₄ Tb ₄	8	-4.382	-4.471	-3.000e-06	0.00506	0.608	2.063
kag_000_07352	CuNi ₃ Tm ₂	6	-5.231	-5.273	0.0000e+00	0.00491	0.218	0.968
kag_000_07372	LaNa ₄ Yb ₃	8	-1.654	-1.665	0.0000e+00	0.00381	0.191	0.104

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_07384	Ge ₅ Ru ₇	12	-6.978	-7.353	-1.500e-05	0.00457	1.312	1.111
kag_000_07414	CaCdLaNd ₄ Pb	8	-3.813	-3.959	0.000e+00	0.00798	1.894	1.868
kag_000_07444	Co ₄ GePtY	7	-6.364	-6.625	1.000e-06	0.00503	0.454	0.424
kag_000_07473	Co ₅ GePt ₂	8	-6.263	-6.413	-5.300e-05	0.0087	0.461	0.425
kag_000_07478	CaDy ₅ EuTl	8	-3.423	-3.584	-2.000e-06	0.00412	0.533	1.391
kag_000_07480	I ₂ NdRhSn ₂ Tb ₃	9	-3.997	-4.654	-1.000e-06	0.00296	1.185	3.895
kag_000_07498	Al ₂ CaEu ₂ Tb ₃	8	-3.215	-3.459	0.000e+00	0.00635	1.776	1.093
kag_000_07522	Dy ₃ HfLiRhSe ₅ Zn	12	-4.41	-5.505	0.000e+00	0.00728	1.489	3.248
kag_000_07528	CoIrLiMn ₃ O ₆	12	-6.511	-7.07	-5.000e-06	0.00536	0.427	1.145
kag_000_07536	Al ₃ Mn ₃ PtSn	8	-5.509	-5.983	-1.000e-06	0.00945	1.122	2.799
kag_000_07538	Cl ₆ Cs ₂ NbTb ₃	12	-3.816	-4.101	-5.000e-06	0.00813	1.212	2.925
kag_000_07544	GeMn ₄ Ti ₃	8	-7.995	-8.156	-6.000e-06	0.00806	0.705	1.65
kag_000_07584	NdRu ₄ SiU	7	-7.943	-8.585	-4.000e-06	0.00951	0.947	1.469
kag_000_07624	Pt ₅ Ru ₃	8	-7.044	-7.21	0.000e+00	0.00215	0.201	0.172
kag_000_07650	Fe ₃ Ga ₂ GeTb	7	-5.394	-5.771	-6.000e-06	0.00451	0.943	0.739
kag_000_07679	Na ₅ Nd ₃	8	-2.334	-2.33	-1.000e-06	0.00392	0.154	0.109
kag_000_07696	Au ₂ BrCl ₄ Gd ₃	10	-3.359	-4.403	0.000e+00	0.00487	1.728	2.709
kag_000_07698	Dy ₂ MgMn ₃	6	-5.753	-6.026	-3.800e-05	0.00693	0.775	0.777
kag_000_07722	Cs ₃ KYb ₃	7	-0.957	-0.974	-2.900e-06	0.00169	0.327	0.184
kag_000_07760	Dy ₃ Se ₂ Tl ₂	7	-3.75	-4.468	0.000e+00	0.00288	1.481	2.791
kag_000_07766	BiPbTb ₃ Tl	6	-3.915	-4.022	0.000e+00	0.00494	1.504	0.597
kag_000_07775	Dy ₃ Na ₅	8	-2.17	-2.218	0.000e+00	0.00453	0.621	1.189
kag_000_07796	Mn ₃ Ni ₃ P ₂	8	-6.409	-6.914	-3.000e-06	0.00608	0.453	0.471
kag_000_07800	EuIn ₄ Yb ₃	8	-2.194	-2.43	3.000e-06	0.00252	0.72	1.471
kag_000_07822	Gd ₃ Na ₅	8	-2.224	-2.251	-2.000e-06	0.00433	0.588	0.448
kag_000_07826	Na ₅ Nd ₃	8	-2.312	-2.33	-1.050e-04	0.00561	0.299	2.003
kag_000_07834	Tl ₅ Yb ₃	8	-2.016	-2.232	7.000e-06	0.0031	0.818	0.445
kag_000_07851	CaPt ₂ SbTb ₃ Tl	8	-4.35	-5.006	0.000e+00	0.00512	1.587	2.551
kag_000_07864	Ni ₆ RhTi	8	-6.126	-6.177	-1.100e-05	0.00666	0.301	0.806
kag_000_07872	BaBrClGd ₃ IrSnTe	9	-4.065	-5.013	-2.000e-06	0.0049	1.87	2.914
kag_000_07877	BaNa ₄ Tb ₃	8	-2.26	-2.305	3.000e-06	0.00348	1.077	1.714
kag_000_07886	Ga ₂ HfRu ₄	7	-7.33	-7.605	-1.000e-06	0.00491	0.515	0.854
kag_000_07912	Co ₄ GeNi ₃	8	-5.906	-6.096	-6.000e-06	0.00452	0.626	1.547
kag_000_07920	AlCaKNa ₂ PdTb ₃	9	-2.952	-3.076	-1.000e-06	0.00263	0.908	1.479
kag_000_07972	InNa ₃ PbTb ₃	8	-3.052	-3.03	-2.000e-06	0.00546	2.049	1.248
kag_000_08011	AlGd ₄ IrNa ₂ Si	9	-4.317	-4.537	-1.000e-06	0.0061	0.802	2.799
kag_000_08014	BiEu ₂ LaNaTb ₃	8	-3.544	-3.529	-2.000e-06	0.00773	0.779	2.041
kag_000_08017	Al ₂ Co ₆	8	-6.297	-6.34	-2.000e-06	0.00584	0.208	0.739
kag_000_08088	K ₃ SnYb ₃	7	-1.393	-1.594	-3.200e-05	0.00645	0.855	2.834
kag_000_08119	AgNd ₃ S ₈	12	-4.377	-5.255	1.000e-06	0.00431	2.588	3.006
kag_000_08153	Cl ₄ Gd ₃ SnTi ₂	10	-4.235	-4.985	-6.000e-06	0.0056	1.609	2.085
kag_000_08159	Dy ₅ Sn ₂ Yb	8	-4.171	-4.363	0.000e+00	0.00378	1.449	0.957
kag_000_08173	Co ₃ Dy ₃ HfHoSi ₄	12	-5.848	-6.331	-2.300e-04	0.0089	0.828	1.365
kag_000_08179	Fe ₃ Pt ₅	8	-6.585	-6.739	-1.400e-05	0.00618	0.348	0.432
kag_000_08193	RhRu ₇	8	-8.329	-8.901	1.000e-06	0.00371	0.748	0.564
kag_000_08196	Co ₅ GaNi ₂	8	-6.05	-6.07	-3.000e-06	0.0049	0.148	0.688
kag_000_08222	AsBaNd ₃ Te ₂ Tl	8	-4.217	-4.744	1.000e-06	0.00309	1.156	2.136
kag_000_08224	CuGa ₄ Ni ₃	8	-3.821	-4.162	-3.000e-06	0.00612	0.332	0.33
kag_000_08231	Dy ₃ NdSb ₂ ScTe ₃ Tm	11	-4.14	-5.213	-1.000e-06	0.00549	1.961	2.136
kag_000_08242	Pd ₂ Pt ₂ Ru ₃ Sn	8	-6.676	-6.74	5.000e-06	0.00546	0.323	0.268
kag_000_08290	Al ₂ CaDy ₃ LuSr	8	-3.513	-3.688	-6.000e-06	0.00474	2.165	3.287
kag_000_08293	Co ₂ Ni ₆	8	-5.711	-5.736	0.000e+00	0.00415	0.115	0.099

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_08311	AgNi ₃ ScSe ₃	8	-4.144	-4.904	3.000e-06	0.00935	1.145	1.05
kag_000_08331	BaCaGeNa ₅ SrTb ₃	12	-2.268	-2.485	0.000e+00	0.00361	1.645	1.102
kag_000_08339	Mn ₄ Ni ₃ Si	8	-7.202	-7.312	-2.000e-06	0.00747	0.301	0.88
kag_000_08349	AlCo ₂ CrMn ₃ Ni	8	-7.324	-7.434	-7.000e-06	0.00767	0.221	0.742
kag_000_08353	K ₃ NaSnYb ₃	8	-1.362	-1.544	4.000e-06	0.00673	2.074	1.735
kag_000_08355	Co ₄ Fe ₈	12	-7.582	-7.676	-3.000e-06	0.00607	0.189	0.184
kag_000_08361	Ge ₂ MnNi ₄ Si ₂ Ti	10	-5.754	-6.026	-1.000e-06	0.00714	0.326	1.083
kag_000_08374	Fe ₃ Ni ₄ Pt	8	-6.321	-6.417	-3.000e-06	0.00513	0.268	0.205
kag_000_08382	Al ₂ CoGd ₃ S ₅ Ti	12	-4.923	-5.7	-5.800e-05	0.00814	0.661	1.912
kag_000_08393	Dy ₃ Tl ₅	8	-3.17	-3.292	-2.000e-06	0.00503	0.865	2.194
kag_000_08408	AlPt ₂ Ru ₅	8	-7.597	-7.892	0.000e+00	0.00493	0.66	0.44
kag_000_08417	Fe ₃ Ni ₈ V	12	-6.34	-6.397	2.000e-06	0.00639	0.198	0.155
kag_000_08437	CsNd ₃ S ₃ Si	8	-4.331	-5.356	-1.100e-05	0.00438	2.444	4.497
kag_000_08443	Al ₃ GeMn ₃	7	-5.887	-6.127	-2.000e-06	0.00817	0.373	0.388
kag_000_08453	EuNa ₂ Yb ₅	8	-1.415	-1.421	-3.000e-06	0.00406	0.151	0.131
kag_000_08478	GaIrMn ₃ Zr ₂	7	-7.852	-8.126	0.000e+00	0.00783	1.053	1.295
kag_000_08485	MgNd ₃ SnSrTl ₂	8	-3.304	-3.499	-2.000e-06	0.00374	1.132	2.294
kag_000_08501	Co ₄ Ge ₂ SiY ₃	10	-6.336	-6.474	-6.000e-06	0.00525	0.241	0.286
kag_000_08533	In ₂ LuTb ₄ Tl	8	-3.864	-4.038	1.000e-06	0.00377	1.361	4.107
kag_000_08543	Fe ₃ Sn ₄	7	-4.642	-5.295	0.000e+00	0.00999	1.264	1.055
kag_000_08565	Pt ₄ Ru ₃ U	8	-7.789	-8.12	-1.000e-06	0.00669	0.371	0.361
kag_000_08567	PrRu ₄ Th	6	-8.3	-8.383	-4.000e-06	0.00812	0.236	0.106
kag_000_08571	Dy ₃ Na ₅	8	-2.141	-2.217	-2.300e-05	0.00333	0.537	0.237
kag_000_08591	Al ₄ MgMnNi ₄ TiZn	12	-4.776	-4.944	-1.200e-05	0.00931	0.589	0.729
kag_000_08595	Au ₃ Br ₅ Dy ₃ Pd	12	-3.33	-4.093	1.000e-06	0.00296	0.924	3.928
kag_000_08607	Gd ₃ LuTl ₄	8	-3.284	-3.619	1.000e-06	0.00674	0.873	0.411
kag_000_08619	As ₂ Gd ₃ PbSr	7	-4.068	-4.852	0.000e+00	0.00787	0.998	2.4
kag_000_08624	BrNaPb ₂ Tb ₃ U	8	-4.908	-4.5	-8.000e-06	0.00534	2.183	2.548
kag_000_08627	Er ₂ Ni ₂ Ru ₃	7	-6.564	-6.795	-5.270e-04	0.00945	0.377	0.242
kag_000_08636	KNaSn ₃ Yb ₃	8	-2.323	-2.594	-1.000e-06	0.00248	0.694	0.572
kag_000_08649	CaCd ₂ EuInTb ₃	8	-2.796	-2.919	1.000e-06	0.00542	0.771	0.558
kag_000_08652	Na ₅ Yb ₃	8	-1.254	-1.276	-3.000e-06	0.00311	0.398	1.166
kag_000_08656	Co ₂ Mn ₄ Tc ₂	8	-8.639	-8.749	-3.700e-05	0.00451	0.17	0.132
kag_000_08657	LaNd ₄ SbSnTl	8	-4.363	-4.765	-1.000e-05	0.00698	1.835	0.998
kag_000_08658	BaDy ₃ Na ₃ Sr	8	-2.275	-2.337	-7.000e-06	0.0022	1.452	2.643
kag_000_08676	Co ₂ KS _n Yb ₃	10	-3.446	-3.708	-1.000e-06	0.00486	1.052	0.956
kag_000_08681	Ce ₂ Nd ₃ Sn ₂ Yb	8	-4.31	-4.626	-1.200e-05	0.00964	1.225	0.81
kag_000_08693	Co ₃ CrPtZr ₂	7	-7.664	-7.942	-1.000e-06	0.00566	0.313	1.225
kag_000_08720	Dy ₃ Hg ₇ LaSb	12	-2.202	-2.363	-3.000e-06	0.00782	1.499	1.176
kag_000_08721	As ₂ Br ₅ Dy ₃ LiMn	12	-3.532	-4.348	-1.100e-05	0.00827	1.717	2.93
kag_000_08749	AuMgMn ₃ TiZn	7	-5.477	-5.799	-5.000e-06	0.00996	0.416	0.278
kag_000_08752	Gd ₃ Sn ₄ Sr	8	-4.058	-4.29	0.000e+00	0.00558	0.968	1.41
kag_000_08788	Eu ₂ Sb ₃ Sn ₄ Tb ₃	12	-4.096	-4.351	1.000e-06	0.0086	1.361	1.034
kag_000_08801	CaEuKNa ₂ Nd ₃	8	-2.394	-2.448	8.000e-06	0.00409	1.34	3.412
kag_000_08822	Fe ₃ NiTh ₂	6	-7.539	-7.551	0.000e+00	0.00448	0.088	0.082
kag_000_08838	K ₂ Sr ₂ Tb ₃ Tl	8	-2.288	-2.457	-1.000e-06	0.00961	1.394	3.379
kag_000_08839	EuIn ₂ La ₂ Tb ₃	8	-3.913	-4.021	0.000e+00	0.00773	1.39	2.182
kag_000_08867	Cs ₃ Dy ₃	6	-1.831	-2.035	-7.000e-06	0.00227	0.64	1.955
kag_000_08880	CoCrGa ₂ Mn ₄	8	-7.074	-7.208	-5.900e-05	0.00674	0.63	1.435
kag_000_08881	Eu ₂ Gd ₄ Sr ₂	8	-2.801	-2.972	-1.000e-06	0.0036	1.185	1.545
kag_000_08913	Fe ₄ LaSc	6	-7.175	-7.193	-6.000e-06	0.00694	0.072	0.103
kag_000_08926	Cs ₃ Tb ₃	6	-1.835	-2.051	5.000e-06	0.00283	0.969	2.041

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_08936	BaGd ₄ Tl ₃	8	-3.253	-3.521	2.000e-06	0.00318	0.793	1.309
kag_000_08944	Br ₅ Dy ₃ MnTi	10	-3.947	-4.654	0.000e+00	0.00514	0.48	2.606
kag_000_08950	AsFe ₄ Pt ₃	8	-6.619	-6.838	-7.000e-06	0.00732	0.638	0.408
kag_000_08963	Co ₃ Ga ₄ Ni	8	-4.806	-4.875	-5.000e-06	0.00591	0.318	0.207
kag_000_08964	BaGaNaSnSrYb ₃	8	-2.099	-2.194	-6.000e-06	0.00194	0.757	0.347
kag_000_08984	Au ₂ Co ₅ La	8	-5.121	-5.603	-2.100e-05	0.00481	0.404	1.955
kag_000_08992	AlCo ₂ CrFe ₃ Ga	8	-6.73	-6.792	-7.000e-06	0.0072	0.204	0.86
kag_000_09004	Co ₄ Ni ₄	8	-6.031	-6.076	-2.900e-05	0.00488	0.253	0.153
kag_000_09008	Gd ₃ I ₄ NbTl	9	-3.451	-3.979	-1.000e-06	0.00216	1.491	1.966
kag_000_09037	Co ₄ Ga ₂ NiTi	8	-6.066	-6.136	1.000e-06	0.00825	0.262	0.766
kag_000_09046	Br ₂ ClIMoTb ₃	8	-3.996	-4.566	-7.800e-05	0.00717	1.529	2.288
kag_000_09050	Cl ₄ CsIrTb ₃	9	-3.766	-4.703	-1.000e-06	0.0047	1.403	2.889
kag_000_09065	BiGaIrSnYb ₅	9	-3.169	-3.507	-1.000e-06	0.00341	2.202	3.468
kag_000_09076	Al ₂ Mn ₃ Pt ₃	8	-6.765	-6.847	-1.000e-06	0.00682	0.206	0.932
kag_000_09084	CaNa ₄ Tb ₃	8	-2.327	-2.352	-3.000e-06	0.00442	0.628	0.352
kag_000_09087	Br ₅ PdTb ₃ Tl	10	-3.147	-4.066	-1.000e-06	0.00569	1.273	2.331
kag_000_09093	ErFe ₄ SnU	7	-7.11	-7.457	-1.000e-06	0.00919	0.541	1.103
kag_000_09096	Fe ₃ Mn ₂ Ni ₃	8	-7.022	-7.234	-1.200e-05	0.00855	0.65	0.483
kag_000_09097	CaGaNa ₂ Nd ₃ Sn	8	-3.184	-3.383	1.000e-06	0.00779	1.015	0.675
kag_000_09108	HCoGePt ₂ Ru ₃	8	-6.468	-6.699	-3.000e-06	0.00808	0.132	0.321
kag_000_09154	AsBiBrNaYb ₃	7	-2.351	-3.168	0.000e+00	0.00326	2.556	3.698
kag_000_09162	Al ₃ CoFe ₇ Ti	12	-6.896	-6.98	-7.000e-06	0.00825	0.191	0.25
kag_000_09190	Co ₆ PtRh	8	-6.399	-6.76	-7.000e-06	0.00514	0.822	1.038
kag_000_09192	Na ₂ SrTl ₂ Yb ₃	8	-1.637	-1.769	1.000e-06	0.00178	1.689	2.602
kag_000_09198	Cs ₃ Nd ₃	6	-1.982	-2.167	-2.000e-06	0.00165	1.312	1.437
kag_000_09216	FeMn ₃ Rh ₃ Ti	8	-8.066	-8.186	-3.000e-06	0.00408	0.124	1.411
kag_000_09240	CsEuGeIrNaYb ₄	9	-2.518	-2.719	-1.000e-06	0.00512	1.375	1.063
kag_000_09265	CaICoRh ₃ Ru ₃	9	-7.289	-7.784	-6.000e-06	0.00439	0.508	0.3
kag_000_09268	AlAs ₂ Fe ₅	8	-6.381	-6.707	-9.000e-06	0.00416	1.101	1.896
kag_000_09287	Cl ₅ Nd ₃ Ti ₄	12	-4.389	-5.343	-6.800e-05	0.00932	1.977	3.641
kag_000_09295	BeCe ₂ Ge ₂ Mn ₅	10	-6.715	-6.992	1.000e-06	0.00546	0.949	0.579
kag_000_09304	Ga ₃ Ni ₃ Pt	7	-4.522	-4.626	0.000e+00	0.00536	0.282	0.326
kag_000_09306	Ca ₂ Dy ₃ Na ₃	8	-2.355	-2.416	-3.000e-06	0.00311	0.694	0.524
kag_000_09319	BaCaGa ₂ Gd ₃ Tl	8	-3.302	-3.416	0.000e+00	0.00651	0.328	0.573
kag_000_09322	SiSnTb ₃ Tl ₄	9	-3.464	-3.77	-6.000e-06	0.00572	1.29	2.604
kag_000_09375	MnNi ₇	8	-5.754	-5.815	-6.000e-06	0.00844	0.184	1.395
kag_000_09386	Dy ₅ Ga ₄ Ir ₃	12	-5.151	-5.683	-1.000e-06	0.0056	1.166	1.8
kag_000_09397	Gd ₃ Na ₄ Tl	8	-2.439	-2.49	-1.000e-06	0.00371	1.136	1.053
kag_000_09454	BrISnTb ₃ Tl	7	-3.003	-3.847	-3.000e-06	0.0048	1.731	2.429
kag_000_09469	Cl ₄ Tb ₃ Tl	8	-3.721	-4.136	-1.000e-06	0.00476	0.819	2.434
kag_000_09483	Co ₃ HoNSm	6	-5.554	-6.75	-6.000e-06	0.00997	1.469	1.666
kag_000_09493	Dy ₄ LaNaNdSn	8	-4.102	-4.19	-1.000e-06	0.00428	1.316	3.688
kag_000_09496	Fe ₄ Ni ₄	8	-6.453	-6.652	-1.640e-04	0.00587	0.251	0.793
kag_000_09516	CeCuGaMgNi ₆ Os ₂	12	-5.651	-5.792	1.000e-06	0.00998	0.372	0.557
kag_000_09541	Ba ₂ Ru ₃ Zn ₆	11	-2.974	-3.31	7.000e-06	0.00587	1.089	1.404
kag_000_09594	CaEu ₂ Na ₂ Nd ₃	8	-2.606	-2.662	-1.000e-06	0.00339	1.044	2.689
kag_000_09619	EuGe ₂ Ni ₅	8	-4.567	-5.172	-1.000e-06	0.00596	1.119	2.864
kag_000_09640	Co ₃ GeMnNi ₇	12	-5.874	-6.026	-1.300e-05	0.00599	0.534	0.393
kag_000_09644	DyEu ₂ InNd ₄	8	-3.755	-3.758	0.000e+00	0.00565	0.102	0.079
kag_000_09651	Co ₃ Pt ₅	8	-6.258	-6.328	-3.000e-06	0.00243	0.219	0.227
kag_000_09672	Bi ₃ Ni ₃	6	-3.578	-4.546	-6.000e-06	0.00504	0.967	0.471
kag_000_09693	EuGd ₃ InLuSn ₂	8	-3.979	-4.234	-2.000e-06	0.00909	1.4	1.594

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_09709	Al ₅ EuGaNdPrRu ₃	12	-5.008	-5.375	2.000e-06	0.00616	0.608	0.661
kag_000_09742	Cr ₂ Gd ₃ S ₄ Sn ₃	12	-4.605	-5.763	-4.000e-06	0.00542	1.418	2.008
kag_000_09746	Gd ₃ I ₅ Pt	9	-3.327	-4.053	-3.000e-06	0.00592	0.861	2.921
kag_000_09749	CaKNa ₃ Tb ₃	8	-2.146	-2.218	-1.800e-05	0.00205	1.121	0.777
kag_000_09766	AgAl ₂ AuCo ₃ Sr	8	-4.274	-4.575	-4.900e-05	0.00646	0.453	0.296
kag_000_09770	Ga ₂ Ge ₃ Ni ₇	12	-4.972	-5.064	-2.000e-05	0.0077	1.003	0.787
kag_000_09772	Fe ₄ LiOsRh ₂	8	-7.198	-7.324	-1.000e-06	0.00674	0.351	0.269
kag_000_09792	K ₂ Tl ₂ Yb ₃	7	-1.411	-1.622	-3.000e-06	0.00381	1.181	1.945
kag_000_09825	Al ₃ Co ₂ Mg ₂ Mn ₃ Zr ₂	12	-5.935	-6.2	-2.000e-06	0.00364	0.585	0.557
kag_000_09853	Fe ₇ Ni ₄ Ti	12	-7.103	-7.197	2.000e-06	0.00542	0.315	0.296
kag_000_09858	Gd ₃ Na ₅	8	-2.233	-2.249	-2.300e-05	0.00133	0.256	1.026
kag_000_09869	ErHf ₂ Ru ₄	7	-8.785	-8.965	4.000e-06	0.00798	0.153	0.451
kag_000_09877	CaEuLaNa ₂ Yb ₃	8	-1.816	-1.866	0.000e+00	0.00308	1.607	2.705
kag_000_09904	Al ₂ Ru ₃ Sm ₂	7	-6.061	-6.55	-1.000e-06	0.00719	0.867	0.766
kag_000_09946	Al ₃ CrMn ₅ Zr ₃	12	-7.503	-7.735	-1.100e-05	0.00713	0.476	1.44
kag_000_09953	Br ₄ CsIrTb ₃	9	-3.631	-4.355	9.000e-06	0.00789	1.606	2.751
kag_000_09978	Co ₃ FeGePtSn	7	-5.926	-6.127	-8.000e-05	0.00987	0.637	1.884
kag_000_10000	Br ₅ Nd ₃ Ti ₃ V	12	-4.303	-5.065	-2.000e-06	0.00496	0.842	3.022
kag_000_10021	Al ₂ HfMgMn ₃	7	-6.258	-6.571	-1.000e-06	0.00591	0.67	1.251
kag_000_10041	Na ₅ Tb ₃	8	-2.196	-2.235	0.000e+00	0.00219	0.586	0.286
kag_000_10051	SnTl ₄ Yb ₃	8	-2.083	-2.521	-1.000e-06	0.00335	2.0	2.643
kag_000_10062	EuGd ₃ IrrNaOTe	9	-4.245	-4.952	-2.000e-06	0.0088	1.508	3.127
kag_000_10114	Dy ₃ PbTe ₂ Tl	7	-3.869	-4.353	-3.000e-06	0.00407	1.477	2.137
kag_000_10138	Eu ₂ Ga ₃ Gd ₃	8	-3.361	-3.625	-1.000e-06	0.00456	0.701	1.371
kag_000_10176	EuGd ₄ NaTl ₂	8	-3.133	-3.382	0.000e+00	0.00586	1.386	1.734
kag_000_10188	AlMn ₃ Pt ₄	8	-6.95	-7.078	0.000e+00	0.00468	0.191	1.442
kag_000_10208	AlErMn ₃ Si ₂	7	-6.434	-6.657	-2.000e-06	0.00869	0.487	0.354
kag_000_10218	BrCaGd ₃ I ₃	8	-3.066	-3.476	1.000e-06	0.00446	1.234	2.034
kag_000_10224	Ge ₂ Ru ₃ SnTl ₂	8	-4.57	-5.366	0.000e+00	0.00782	1.229	2.107
kag_000_10230	Ga ₄ Mn ₃ Sr	8	-4.843	-5.043	-1.000e-06	0.00363	0.341	0.289
kag_000_10240	Al ₂ CeNi ₄ Sn	8	-4.582	-5.255	0.000e+00	0.00833	1.042	1.859
kag_000_10273	CaGd ₃ INaSe ₂	8	-3.264	-4.002	3.000e-06	0.00742	2.258	2.482
kag_000_10281	EuInSe ₃ Tb ₃	8	-4.13	-4.744	-5.000e-06	0.00392	1.151	2.072
kag_000_10285	BaEuTl ₂ Yb ₄	8	-1.862	-1.983	-1.900e-05	0.00461	1.044	0.884
kag_000_10290	Co ₄ Pr ₂	6	-6.165	-6.233	-1.100e-05	0.0057	0.194	0.166
kag_000_10311	MgNi ₆ Si	8	-5.088	-5.177	-2.000e-06	0.00885	0.532	0.491
kag_000_10321	PtRu ₆ Zr	8	-8.456	-8.826	-1.000e-06	0.00734	0.683	1.114
kag_000_10324	Ni ₄ Sn ₆	10	-4.392	-4.563	0.000e+00	0.00461	0.572	0.769
kag_000_10325	K ₄ NaYb ₃	8	-0.981	-1.075	-1.600e-05	0.00753	1.447	1.167
kag_000_10330	Ga ₃ PtRu ₄	8	-6.466	-6.604	6.000e-06	0.0032	0.798	1.814
kag_000_10341	Eu ₂ Na ₃ Nd ₃	8	-2.523	-2.55	-1.000e-06	0.00362	0.328	0.315
kag_000_10342	EuTb ₃ Tl ₄	8	-3.231	-3.319	-5.000e-06	0.00306	0.759	0.386
kag_000_10344	Gd ₅ ORuSnSr	9	-4.716	-5.488	3.000e-06	0.00458	1.408	3.302
kag_000_10352	EuGd ₃ In ₃ Lu	8	-3.621	-3.787	-2.000e-06	0.00282	0.636	0.411
kag_000_10362	BaSe ₂ Tb ₃ Tl	7	-3.58	-4.517	-3.000e-06	0.00545	1.267	2.239
kag_000_10373	Cl ₃ Nd ₃ RbSn	8	-3.172	-4.243	3.000e-06	0.00776	1.766	2.353
kag_000_10382	Ga ₂ Gd ₅ Tl	8	-4.025	-4.162	2.000e-06	0.00551	0.58	1.095
kag_000_10388	Fe ₆ Ni ₂	8	-6.998	-7.347	-7.000e-06	0.00732	0.743	0.555
kag_000_10397	Br ₂ Cl ₃ Pd ₂ Tb ₃	10	-3.71	-4.67	0.000e+00	0.00452	1.699	2.895
kag_000_10400	Fe ₃ Ni ₂ Pt ₂	7	-6.353	-6.496	-3.000e-06	0.00665	0.338	1.194
kag_000_10409	DyNaNdSbTb ₄	8	-4.005	-4.254	-1.000e-06	0.00409	1.659	1.515
kag_000_10458	CoMn ₆ Ni	8	-8.011	-8.264	3.000e-06	0.00439	0.48	0.976

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_10473	CBGeMn ₄ Pt ₂ Ti	10	-7.405	-7.768	1.000e-06	0.00798	0.918	2.769
kag_000_10508	Ce ₂ Ru ₄	6	-7.754	-8.406	-1.000e-06	0.00296	0.485	0.297
kag_000_10537	Hf ₂ Ru ₄	6	-9.714	-9.826	-2.000e-06	0.00334	0.281	0.221
kag_000_10551	Ga ₄ Ni ₃	7	-4.023	-4.298	-6.400e-05	0.00634	0.459	0.657
kag_000_10557	Tb ₃ Tl ₅	8	-3.207	-3.312	8.000e-06	0.00615	0.448	1.277
kag_000_10576	Lu ₄ Ru ₃	7	-6.275	-6.626	3.000e-06	0.00558	0.438	0.326
kag_000_10582	Co ₃ Zr ₄	7	-7.972	-8.001	-1.000e-05	0.00964	0.103	0.065
kag_000_10592	Br ₃ Cs ₂ Gd ₃ Pt	9	-3.189	-3.704	-2.000e-06	0.00476	0.672	2.432
kag_000_10610	BaSn ₈ Tb ₃	12	-4.047	-4.253	-9.000e-05	0.00918	0.954	1.037
kag_000_10616	Br ₂ SnYb ₃	6	-2.145	-3.1	0.000e+00	0.004	2.292	4.014
kag_000_10625	Fe ₄ SiZr ₂	7	-7.743	-7.969	1.000e-06	0.00677	0.256	0.483
kag_000_10634	Dy ₃ In ₂ LuNa ₂	8	-3.206	-3.227	-1.000e-06	0.00829	0.312	0.223
kag_000_10635	Co ₃ Ni ₇ Ta	11	-6.273	-6.435	-4.000e-06	0.0069	0.297	0.905
kag_000_10662	AlCoMn ₄ PtSi	8	-7.119	-7.402	-1.700e-05	0.00734	0.393	0.87
kag_000_10681	Co ₄ NdTb	6	-6.233	-6.313	-1.000e-05	0.00432	0.146	0.138
kag_000_10684	AlNi ₇	8	-5.229	-5.451	-4.700e-05	0.00445	0.301	0.218
kag_000_10686	Ni ₄ PtZr ₂	7	-6.594	-6.75	-6.000e-06	0.00982	0.255	1.067
kag_000_10697	FeNi ₈ Rh ₂ Ti	12	-6.129	-6.247	6.000e-06	0.0072	0.829	0.71
kag_000_10707	In ₄ RbYb ₃	8	-2.18	-2.087	-1.000e-06	0.00245	0.598	2.203
kag_000_10717	AuKSe ₃ Tb ₃	8	-3.972	-4.876	-1.000e-06	0.00434	1.388	4.526
kag_000_10724	Ce ₂ Gd ₃ Na ₂ Sn	8	-3.851	-3.897	-3.710e-04	0.00523	0.392	1.164
kag_000_10747	Ba ₂ Tb ₃ Tl ₂	7	-3.03	-3.254	0.000e+00	0.00445	0.613	0.851
kag_000_10751	Eu ₃ InTb ₃	7	-2.93	-3.138	-1.000e-06	0.00584	0.999	3.643
kag_000_10770	Eu ₃ NaTb ₃ Tl	8	-2.642	-2.812	3.000e-06	0.00241	0.866	3.125
kag_000_10776	Gd ₅ Sn ₃	8	-4.656	-4.823	0.000e+00	0.00295	0.622	0.347
kag_000_10788	Co ₄ Sn ₅ Sr	10	-4.88	-4.996	2.000e-06	0.00885	0.487	0.481
kag_000_10794	AlEuGd ₃ PbSb	7	-3.984	-4.355	-1.000e-06	0.00842	0.913	2.293
kag_000_10799	Dy ₂ Ru ₄ Zn	7	-6.219	-6.826	-3.000e-06	0.00404	0.664	0.859
kag_000_10800	EuNa ₄ Tb ₃	8	-2.254	-2.32	-5.000e-06	0.00504	0.562	1.19
kag_000_10808	CuMn ₄ Ni ₆ Sc	12	-6.342	-6.536	2.000e-06	0.00841	0.762	0.596
kag_000_10815	Co ₆ PtZn	8	-5.945	-6.03	-3.000e-06	0.00687	0.194	0.153
kag_000_10839	Mn ₄ Pt ₃ Si	8	-7.275	-7.509	-1.000e-06	0.0049	0.552	0.434
kag_000_10840	In ₂ Na ₂ Yb ₄	8	-1.902	-1.835	1.000e-06	0.00548	0.784	2.147
kag_000_10881	Co ₅ Ni ₂ Si	8	-6.382	-6.492	-1.000e-06	0.00551	0.392	1.476
kag_000_10883	GaPt ₄ Ru ₃	8	-6.597	-6.943	1.000e-06	0.00658	0.079	0.959
kag_000_10898	AlNi ₄ SnZr	7	-5.442	-5.734	-3.000e-06	0.00734	0.354	1.756
kag_000_10912	Rh ₃ Ru ₄ Zr	8	-8.524	-8.577	-1.000e-06	0.0032	0.199	0.171
kag_000_10946	Co ₃ Ni ₅	8	-5.819	-5.9	3.000e-06	0.00644	0.276	0.22
kag_000_10960	Br ₅ IrTb ₃	9	-3.707	-4.84	-2.000e-06	0.00931	1.642	2.395
kag_000_10977	DyMgRu ₄	6	-7.172	-7.254	-2.000e-06	0.00668	0.283	0.192
kag_000_10996	EuMgNd ₄ SmZn	8	-3.411	-3.478	-4.000e-06	0.00282	0.428	0.315
kag_000_11010	CrDy ₃ Se ₈	12	-5.096	-5.29	-2.800e-05	0.00525	0.985	0.447
kag_000_11043	Co ₁₁ Ti	12	-6.997	-7.044	2.000e-06	0.00682	0.129	0.136
kag_000_11067	Br ₅ Cu ₂ Gd ₃ MnRu	12	-3.879	-4.485	-1.000e-06	0.00851	0.96	2.707
kag_000_11129	CsRbSbSnYb ₃	7	-2.025	-2.269	0.000e+00	0.00513	1.605	2.806
kag_000_11193	Na ₂ Nd ₃ Tl ₃	8	-2.962	-3.056	-2.000e-06	0.00748	0.554	0.465
kag_000_11227	Br ₅ Gd ₃ Rh ₂	10	-3.923	-4.572	-6.000e-06	0.00636	1.87	2.605
kag_000_11229	Na ₅ Nd ₃	8	-2.295	-2.328	-2.000e-06	0.003	0.237	0.354
kag_000_11247	Nd ₃ Rb ₂ SnTl	7	-2.717	-3.151	2.000e-06	0.00399	1.304	2.455
kag_000_11252	Dy ₃ Sn ₂ TeTl	7	-3.977	-4.273	-1.000e-06	0.00607	0.97	2.532
kag_000_11282	Ga ₃ GeNi ₄	8	-4.421	-4.55	-1.000e-06	0.00967	0.593	0.997
kag_000_11283	Ni ₃ Sn ₆	9	-3.633	-4.37	0.000e+00	0.00867	1.191	1.328

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_11294	Al ₄ FeNi ₃ Yb ₄	12	-3.977	-4.093	-1.000e-06	0.00263	0.492	0.472
kag_000_11304	Co ₃ Mn ₃ RuTi	8	-7.948	-8.081	1.700e-05	0.00693	0.573	2.292
kag_000_11309	Cs ₃ Tb ₃	6	-1.673	-2.055	-1.400e-05	0.00204	2.546	1.833
kag_000_11326	Ni ₅ Pt ₂ Rh	8	-5.808	-5.837	-2.000e-06	0.00667	0.151	0.756
kag_000_11362	Br ₄ IRh ₂ Tb ₃	10	-4.008	-4.708	-2.000e-06	0.00618	1.054	2.691
kag_000_11374	Gd ₃ NbRu ₂ Se ₅ Ti	12	-5.877	-6.353	1.000e-06	0.0062	1.045	2.666
kag_000_11379	CaGd ₄ MgSn ₂	8	-3.688	-4.082	-5.000e-06	0.00441	1.151	0.635
kag_000_11381	Br ₅ RhTb ₃	9	-3.902	-4.531	-1.000e-06	0.00464	0.754	2.595
kag_000_11414	Ge ₂ Ni ₄ SiTi	8	-5.632	-5.835	0.000e+00	0.009	0.374	1.22
kag_000_11440	Fe ₄ NaSn ₄	9	-5.06	-5.173	-2.000e-06	0.00947	0.591	1.465
kag_000_11463	Al ₂ GeNi ₄ U	8	-5.431	-5.865	-1.100e-05	0.00722	1.091	2.246
kag_000_11467	Ni ₃ PtReRh ₂ Ti	8	-7.063	-7.347	-1.200e-05	0.00428	0.423	0.428
kag_000_11483	Gd ₄ In ₄	8	-4.028	-3.933	3.000e-06	0.00175	0.462	1.045
kag_000_11484	Cl ₅ CrGd ₃ Li ₂ Zn	12	-3.402	-3.974	0.000e+00	0.00582	2.376	2.893
kag_000_11498	Tl ₅ Yb ₃	8	-2.024	-2.266	-2.400e-05	0.00499	1.247	1.976
kag_000_11499	Au ₂ IrNi ₃ PrSn	8	-4.503	-5.199	-1.200e-05	0.00943	1.158	1.482
kag_000_11505	Dy ₂ Fe ₄	6	-6.846	-6.931	2.000e-06	0.00643	0.14	1.044
kag_000_11547	As ₃ EuMn ₃ Pt	8	-5.813	-6.427	-1.000e-06	0.00797	2.091	2.28
kag_000_11590	LuNd ₃ Sn ₂ SrTl	8	-3.878	-4.076	1.000e-06	0.00762	1.635	0.795
kag_000_11594	Pt ₄ Ru ₄	8	-7.526	-7.585	-3.000e-06	0.00596	0.14	0.089
kag_000_11599	Mn ₄ Ni ₂ Si ₂ Ta ₄	12	-8.966	-9.18	-2.000e-05	0.00897	0.394	0.386
kag_000_11623	BiDy ₃ EuLa ₅ PbSr	12	-4.021	-4.223	-3.000e-06	0.00549	0.667	0.582
kag_000_11664	LaTl ₄ Yb ₃	8	-2.36	-2.62	-2.300e-05	0.00791	1.301	1.679
kag_000_11685	CaKNd ₃ SrTl ₂	8	-2.627	-2.958	-1.000e-06	0.00311	2.213	3.26
kag_000_11688	Co ₄ Sc ₂	6	-6.993	-7.114	0.000e+00	0.00566	0.19	0.199
kag_000_11689	Cs ₃ Yb ₃	6	-0.824	-0.844	-3.600e-06	0.00232	0.402	0.272
kag_000_11695	Fe ₄ GaGePd ₂	8	-6.04	-6.196	-4.000e-06	0.00436	0.713	0.415
kag_000_11696	AlFe ₃ GaSc ₂	7	-6.267	-6.385	-3.000e-06	0.00716	0.313	0.201
kag_000_11699	AuNd ₄ PtS ₂ SbSi ₃	12	-4.78	-5.55	0.000e+00	0.00466	2.019	2.371
kag_000_11725	Ni ₂ RhRu ₃ SnZn	8	-6.193	-6.233	0.000e+00	0.00528	0.25	0.298
kag_000_11739	Fe ₅ Pt ₃	8	-6.829	-7.238	-6.000e-06	0.00647	0.564	0.653
kag_000_11741	Eu ₃ Gd ₃ SnSr	8	-3.106	-3.164	-7.000e-06	0.00517	0.451	2.17
kag_000_11768	Al ₂ Fe ₄ Ga ₂ Nb ₃ Ta	12	-7.541	-7.633	-6.000e-06	0.00552	0.285	0.304
kag_000_11780	BiCeEuGd ₅	8	-4.539	-4.451	-9.500e-05	0.00511	0.546	0.393
kag_000_11805	Co ₃ Pt ₅	8	-5.927	-6.321	-5.600e-05	0.00515	0.513	1.689
kag_000_11854	Co ₃ PdSnTiZr	7	-6.754	-6.888	0.000e+00	0.00623	0.37	0.307
kag_000_11865	Al ₂ PdPtRu ₄	8	-6.957	-7.214	3.000e-06	0.00484	0.398	0.355
kag_000_11868	GaGeNi ₃ Pt ₂ Si	8	-4.836	-5.482	-5.000e-06	0.00794	0.826	0.773
kag_000_11871	Na ₄ SrTb ₃	8	-2.218	-2.282	0.000e+00	0.00207	0.907	0.469
kag_000_11885	AlGe ₂ Pt ₂ Ru ₃	8	-6.488	-6.811	-2.000e-06	0.00501	0.719	2.42
kag_000_11957	AsCo ₂ FeMn ₃ Pt	8	-7.17	-7.359	-2.000e-06	0.00849	0.559	2.222
kag_000_11960	BrNaTb ₃ Tl ₃	8	-3.085	-3.228	0.000e+00	0.00452	0.942	3.158
kag_000_11963	Co ₃ FePtTi ₂	7	-7.26	-7.608	-2.500e-05	0.00704	0.64	1.522
kag_000_11972	EuNd ₄ Sn ₃	8	-4.448	-4.553	-2.000e-06	0.00319	0.39	0.31
kag_000_11975	GaGeNi ₆	8	-5.208	-5.232	6.000e-06	0.00725	0.203	0.736
kag_000_11993	CaCdNaNd ₃ RbTl	8	-2.521	-2.55	1.000e-06	0.0048	0.748	1.288
kag_000_12008	Br ₃ SnSrTb ₃	8	-3.251	-4.016	-1.000e-05	0.00358	2.01	3.304
kag_000_12009	Fe ₄ Ru ₄	8	-8.079	-8.533	-1.000e-06	0.00588	0.71	1.145
kag_000_12019	K ₂ Nd ₃ Tl ₂	7	-2.56	-2.894	-1.000e-06	0.0055	1.312	2.223
kag_000_12057	Co ₃ Ni ₅	8	-5.87	-5.899	1.000e-06	0.00292	0.207	0.166
kag_000_12080	Co ₅ Ga ₃	8	-5.52	-5.601	1.000e-05	0.00414	0.645	0.387
kag_000_12095	Pt ₅ Ru ₃	8	-6.994	-7.194	-1.600e-05	0.00532	0.179	0.15

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_12096	Al ₂ GaHo ₃ Mn ₅	11	-6.122	-6.359	-3.000e-06	0.00726	0.431	0.66
kag_000_12148	Rb ₄ Yb ₄	8	-0.712	-0.965	2.000e-07	0.0031	1.769	1.572
kag_000_12183	Mn ₃ Sb ₄ Sc	8	-5.805	-6.162	0.000e+00	0.00485	0.417	0.512
kag_000_12191	BaCdCs ₃ Gd ₃	8	-1.962	-1.993	-1.000e-06	0.00354	0.375	0.325
kag_000_12208	CoMn ₃ OS ₇	12	-5.304	-5.975	0.000e+00	0.00827	0.749	0.668
kag_000_12221	Al ₂ Mn ₃ U ₂	7	-7.628	-8.208	-8.000e-06	0.00771	1.119	0.908
kag_000_12238	Fe ₄ MnSi ₂ Ti	8	-7.519	-7.798	-1.000e-06	0.00466	0.978	0.719
kag_000_12239	Pt ₄ Ru ₄	8	-7.362	-7.601	-5.000e-06	0.00286	0.326	0.173
kag_000_12249	Dy ₄ Ni ₃	7	-4.267	-5.185	-2.000e-05	0.00649	1.072	1.055
kag_000_12253	Dy ₃ EuIn ₂ Pr ₂	8	-3.881	-3.97	-1.000e-06	0.00433	1.77	1.422
kag_000_12259	BaCaSrTb ₃ Tl ₂	8	-2.901	-3.051	-5.900e-05	0.00604	0.965	1.727
kag_000_12283	Mn ₄ RhSi ₃	8	-7.248	-7.62	-5.000e-06	0.00824	0.803	1.585
kag_000_12292	BaInLu ₂ Nd ₄	8	-3.969	-3.986	3.000e-06	0.00727	0.392	0.232
kag_000_12303	Ga ₅ Ru ₃	8	-5.254	-5.342	2.000e-06	0.00391	0.367	0.308
kag_000_12315	Co ₅ Fe ₂ Ni	8	-6.684	-6.941	4.000e-06	0.00411	0.555	0.309
kag_000_12317	Ga ₂ Pt ₃ Ru ₃	8	-6.51	-6.629	-1.000e-06	0.00953	0.2	0.134
kag_000_12339	GeMn ₄ Pt ₃	8	-7.109	-7.346	-1.000e-06	0.007	0.606	1.113
kag_000_12369	Nd ₄ Te ₄	8	-4.562	-5.347	0.000e+00	0.00599	1.539	2.013
kag_000_12395	Pt ₅ Ru ₃	8	-7.0	-7.196	0.000e+00	0.0061	0.736	1.063
kag_000_12408	Cs ₃ Yb ₄	7	-0.971	-1.023	1.200e-06	0.00628	0.354	0.852
kag_000_12421	CoPtRu ₃ TbTi	7	-7.486	-7.823	-1.100e-05	0.00856	0.215	0.496
kag_000_12428	Tl ₅ Yb ₃	8	-1.921	-2.222	-2.000e-06	0.00438	1.063	1.126
kag_000_12468	Ni ₆ Rh ₂	8	-5.77	-5.849	-1.300e-05	0.00675	0.4	0.267
kag_000_12470	GaMn ₃ Pt ₄	8	-6.732	-6.859	-1.000e-06	0.00739	0.269	2.059
kag_000_12508	MgNi ₃ Y ₂ Zn	7	-4.49	-4.831	-4.000e-06	0.0063	1.566	0.862
kag_000_12510	Mn ₃ Si ₃ Ti ₂	8	-7.433	-7.656	-9.000e-06	0.00562	0.357	0.99
kag_000_12521	Al ₂ Mn ₃ Sb	6	-5.906	-6.282	-6.000e-06	0.00912	0.661	0.651
kag_000_12554	Dy ₂ Fe ₄	6	-6.819	-6.928	-1.400e-05	0.00727	0.368	1.212
kag_000_12615	CoMn ₃ Pt ₄	8	-6.833	-7.199	0.000e+00	0.00626	0.683	0.331
kag_000_12621	AgCaMgNd ₃ SnYb	8	-3.242	-3.452	-2.000e-06	0.00232	1.781	1.678
kag_000_12634	EuIn ₂ Tb ₃ Tl ₂	8	-3.248	-3.435	0.000e+00	0.00551	1.183	0.787
kag_000_12658	Mn ₃ Se ₂ Sn ₂	7	-5.271	-5.723	-3.000e-06	0.00468	1.377	1.276
kag_000_12665	Ba ₂ SbYb ₃	6	-1.944	-2.362	0.000e+00	0.00241	2.408	1.201
kag_000_12679	Fe ₂ I ₅ Nd ₃	10	-3.897	-4.23	3.000e-06	0.00636	1.669	1.787
kag_000_12688	GaGeNi ₆	8	-5.172	-5.233	-7.300e-05	0.00904	0.362	0.344
kag_000_12697	Mn ₃ Sn ₃	6	-5.618	-6.045	0.000e+00	0.00478	0.182	1.108
kag_000_12708	Dy ₃ Ga ₂ Na ₂ Yb	8	-2.742	-2.996	-1.400e-05	0.00479	1.974	1.569
kag_000_12714	BiDy ₃ S ₇	11	-4.977	-5.572	0.000e+00	0.00648	1.497	2.546
kag_000_12727	Ga ₂ Ni ₃ PtU	7	-5.473	-5.997	-5.000e-06	0.00842	0.545	0.446
kag_000_12732	Al ₂ Co ₂ Dy ₃ Se ₅	12	-4.477	-5.227	-2.000e-06	0.00704	1.51	2.484
kag_000_12734	Fe ₃ MgPt ₃ Si	8	-5.946	-6.365	-3.800e-05	0.00906	0.266	2.217
kag_000_12739	Nd ₃ Ni ₄ S ₅	12	-4.989	-5.75	-3.600e-05	0.00647	0.835	2.053
kag_000_12742	Ce ₄ Dy ₄	8	-4.928	-5.134	2.000e-06	0.00637	0.457	1.417
kag_000_12755	NbS ₈ Tb ₃	12	-5.885	-6.111	-7.000e-06	0.00675	1.416	1.191
kag_000_12789	In ₄ Tb ₃ Tl	8	-3.804	-3.563	-1.000e-06	0.00385	0.328	0.287
kag_000_12813	Na ₅ Tb ₃	8	-2.202	-2.233	-3.700e-05	0.00193	0.478	0.318
kag_000_12820	BaNaSbSnTb ₃	7	-3.523	-3.9	-2.000e-06	0.00855	1.456	2.959
kag_000_12835	GaGeIn ₂ Mn ₃	7	-5.137	-5.371	-1.000e-06	0.0087	0.602	0.584
kag_000_12858	Fe ₃ PdPt ₂ Rh ₂	8	-6.751	-6.891	0.000e+00	0.00342	0.259	0.327
kag_000_12859	EuIn ₃ LaTb ₃	8	-3.59	-3.85	2.000e-06	0.00772	0.679	0.446
kag_000_12863	Ga ₃ Mn ₃ Pt ₂	8	-5.884	-6.034	1.500e-05	0.00542	0.46	2.217
kag_000_12884	Co ₃ Mn ₃ NiSn	8	-6.904	-6.944	-4.000e-06	0.00888	0.114	0.767

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_12887	Dy ₃ GaLuNaYb ₂	8	-2.944	-3.089	-1.000e-06	0.00544	1.83	2.558
kag_000_12897	Co ₄ FeThY	7	-6.554	-7.025	-3.000e-06	0.00908	1.042	2.021
kag_000_12913	As ₂ Gd ₆	8	-4.776	-5.053	1.000e-06	0.00209	1.234	0.776
kag_000_12927	Dy ₄ Fe ₈	12	-6.899	-6.934	-9.000e-06	0.00792	0.219	0.253
kag_000_12946	Br ₃ GeMn ₃	7	-4.55	-4.972	-1.000e-06	0.00482	1.005	0.898
kag_000_12948	GeTb ₃ Tl ₃	7	-3.467	-3.86	0.000e+00	0.00348	1.735	1.369
kag_000_12984	EuSr ₂ Tb ₃ Tl ₂	8	-2.777	-2.983	1.000e-06	0.00523	0.806	1.239
kag_000_12990	AlNi ₅ Sn ₂	8	-4.462	-5.053	5.000e-06	0.00708	1.447	2.202
kag_000_13011	BaCa ₂ Na ₂ Tb ₃	8	-2.523	-2.535	-6.000e-06	0.00151	0.701	1.476
kag_000_13031	DyGa ₂ Ru ₃ SbTm	8	-5.773	-6.137	-3.000e-06	0.00985	1.214	1.699
kag_000_13052	GaInPb ₂ Tb ₃	7	-3.636	-4.081	1.000e-06	0.00785	1.924	1.411
kag_000_13074	AlBaDy ₃ EuNdSn	8	-3.687	-3.775	-8.000e-06	0.00605	0.752	3.045
kag_000_13082	Ga ₃ GeRu ₃	7	-5.579	-5.861	-1.100e-05	0.00887	0.274	0.486
kag_000_13084	Dy ₄ Eu ₂ Sn ₂	8	-3.902	-4.055	-2.000e-06	0.00289	1.398	1.157
kag_000_13112	Ga ₆ Gd ₄ MgSn	12	-3.466	-3.838	0.000e+00	0.00545	1.579	1.929
kag_000_13166	Eu ₃ Gd ₃ InTl	8	-2.729	-3.19	-1.000e-06	0.00433	1.944	1.947
kag_000_13168	Cl ₈ MnNd ₃	12	-4.598	-4.769	-2.000e-06	0.0097	0.442	2.826
kag_000_13248	Dy ₃ EuMnSe ₃ Sn	9	-4.403	-5.392	-1.300e-05	0.00545	1.608	3.81
kag_000_13249	CoGaNi ₆	8	-5.378	-5.416	-7.000e-06	0.00457	0.181	0.178
kag_000_13260	Co ₃ NiPt ₃ Ti	8	-6.719	-6.762	-4.000e-06	0.00962	0.109	0.108
kag_000_13268	EuRu ₄ Th	6	-7.616	-7.906	8.000e-06	0.0072	0.34	0.269
kag_000_13317	BaGeSn ₂ TeYb ₃	8	-2.854	-3.288	-4.000e-06	0.0051	2.436	3.29
kag_000_13326	AlFe ₃ Hf ₂	6	-8.262	-8.336	-1.100e-05	0.00499	0.143	0.089
kag_000_13357	Na ₂ Tb ₃ Tl ₃	8	-2.84	-2.971	-5.000e-06	0.00359	0.533	0.514
kag_000_13358	Co ₆ FeV	8	-6.864	-7.386	-5.000e-06	0.00519	0.81	0.352
kag_000_13378	Sn ₄ Tb ₃	7	-4.165	-4.623	-1.000e-06	0.00709	1.314	3.297
kag_000_13382	Al ₄ Fe ₄	8	-5.967	-6.099	-9.000e-06	0.0057	0.474	1.103
kag_000_13384	MgPbTl ₃ Yb ₃	8	-2.031	-2.308	-1.000e-06	0.00522	1.293	2.827
kag_000_13435	AlCoGeNi ₅	8	-5.275	-5.573	2.000e-06	0.0058	0.45	0.925
kag_000_13439	Cl ₃ Cs ₂ Gd ₃ Pt	9	-3.336	-3.975	1.100e-05	0.00785	0.744	2.0
kag_000_13446	Co ₆ Hf ₄ Mn ₂	12	-8.603	-8.678	0.000e+00	0.00585	0.232	0.144
kag_000_13461	Co ₃ Ho ₂ Ni	6	-6.157	-6.187	-6.900e-05	0.00451	0.13	0.055
kag_000_13514	Hf ₄ Ni ₄ P ₄	12	-7.306	-7.957	-3.200e-05	0.0068	1.369	1.208
kag_000_13529	CdGaGd ₃ Sr ₆ Yb	12	-2.222	-2.407	-1.200e-05	0.00665	1.296	0.927
kag_000_13530	Au ₂ S ₅ SnYb ₃	11	-3.389	-4.321	-1.000e-06	0.00319	1.959	2.99
kag_000_13540	BiCs ₃ Tb ₃	7	-2.558	-2.676	-9.000e-06	0.00461	0.569	0.765
kag_000_13541	K ₃ Na ₂ Yb ₃	8	-1.054	-1.12	-2.460e-05	0.00396	0.893	0.631
kag_000_13578	BaEuInNaSnTb ₃	8	-3.281	-3.344	-2.000e-06	0.00599	0.721	0.423
kag_000_13601	Br ₅ Nd ₃ Pt	9	-3.65	-4.534	-2.000e-06	0.00425	1.164	1.856
kag_000_13630	AlCoDy ₆ FeRu ₂	11	-5.542	-5.985	-7.000e-06	0.0046	1.321	1.744
kag_000_13686	CaNa ₃ PbYb ₃	8	-1.729	-1.778	-2.000e-06	0.00432	0.626	2.274
kag_000_13691	FeNi ₇	8	-5.651	-5.705	-3.000e-06	0.00765	0.22	0.16
kag_000_13698	AlBa ₂ Dy ₃ EuInPd ₂	10	-3.695	-3.904	-1.000e-06	0.00637	0.485	1.83
kag_000_13701	AlCaCo ₃ SeSn ₃	9	-4.267	-4.807	0.000e+00	0.00724	0.242	0.786
kag_000_13715	Br ₅ PdTb ₃	9	-3.547	-4.31	-5.000e-06	0.00377	0.627	3.247
kag_000_13725	Gd ₃ Na ₂ SrTl ₂	8	-2.786	-2.891	0.000e+00	0.0031	0.941	3.119
kag_000_13731	Na ₅ Yb ₃	8	-1.28	-1.287	-4.000e-06	0.00198	0.226	1.059
kag_000_13733	CaCeNdSn ₂ Yb ₃	8	-3.286	-3.467	-3.000e-06	0.00281	0.769	0.451
kag_000_13752	BaDy ₃ Sb ₂ Te	7	-4.055	-4.737	1.000e-06	0.00319	1.629	1.658
kag_000_13755	ErFe ₂ HfNi ₃	7	-6.446	-6.757	-7.700e-05	0.00613	0.661	0.449
kag_000_13764	FePt ₃ Ru ₃ Si	8	-7.256	-7.525	-3.000e-06	0.00509	0.418	1.627
kag_000_13791	Ga ₂ Ni ₃ Pt ₃	8	-5.097	-5.433	-8.000e-06	0.00494	1.161	1.139

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_13795	FeGeNi ₆	8	-5.602	-5.723	-4.000e-06	0.00748	0.538	0.947
kag_000_13800	Al ₂ Mn ₄ Sn	7	-6.285	-6.637	2.000e-06	0.00859	0.696	0.601
kag_000_13805	EuHg ₃ Ru ₃	7	-4.002	-4.105	1.000e-06	0.00625	0.248	0.233
kag_000_13811	BaEuGd ₃ NaSrTl	8	-2.638	-2.747	-2.000e-06	0.00849	1.286	2.601
kag_000_13816	Fe ₇ SiZr ₄	12	-8.355	-8.419	-2.000e-05	0.00276	0.166	0.127
kag_000_13826	Co ₄ Tb ₂	6	-6.365	-6.371	-1.400e-05	0.00699	0.069	0.044
kag_000_13856	Cs ₃ TlYb ₃	7	-1.015	-1.203	-6.500e-06	0.00306	1.356	2.812
kag_000_13864	Al ₃ CeMn ₆	10	-7.021	-7.22	-1.000e-06	0.00753	0.241	0.762
kag_000_13870	GeMn ₃ PdSbSn ₃	9	-5.138	-5.63	-4.000e-06	0.00375	0.799	2.01
kag_000_13902	Na ₅ Yb ₃	8	-1.283	-1.287	-1.000e-06	0.00234	0.173	1.034
kag_000_13915	AlFe ₇	8	-7.478	-7.558	1.000e-06	0.00466	0.203	0.747
kag_000_13923	GaNi ₄ SnU	7	-5.578	-5.827	-3.100e-05	0.00531	0.913	1.407
kag_000_13938	Mn ₄ PdPt ₃	8	-7.239	-7.36	-5.000e-06	0.00629	0.186	1.419
kag_000_13941	Fe ₄ Pt ₄	8	-6.796	-7.007	-3.000e-06	0.00505	0.185	0.13
kag_000_13943	CdEuInSr ₂ Tb ₃	8	-2.672	-2.895	1.000e-06	0.00506	1.964	2.483
kag_000_13944	CCoNi ₆ Sn	9	-5.428	-5.781	3.000e-06	0.00832	0.288	1.278
kag_000_13949	La ₂ Ni ₅ Sn ₂	9	-5.072	-5.234	-6.000e-06	0.00645	0.314	0.243
kag_000_13955	Mn ₅ PdPt	7	-7.487	-7.897	0.000e+00	0.00625	0.584	1.306
kag_000_13956	Ga ₂ Ru ₄ Sm	7	-6.515	-6.956	-7.000e-06	0.0058	0.665	0.862
kag_000_13974	CrNi ₇	8	-5.903	-5.914	-2.300e-05	0.00775	0.09	0.141
kag_000_13975	GaNi ₇	8	-5.153	-5.27	0.000e+00	0.0035	0.284	0.772
kag_000_13997	Fe ₂ Ni ₆	8	-5.885	-6.009	-1.000e-06	0.0037	0.643	0.551
kag_000_13999	Fe ₆ Ni ₂	8	-7.053	-7.348	-2.000e-06	0.00534	0.492	0.337
kag_000_14020	Co ₂ GaNi ₅	8	-5.552	-5.566	1.000e-05	0.00633	0.149	0.109
kag_000_14023	Ge ₂ HfMn ₅ Sn ₄	12	-6.529	-6.57	-2.000e-06	0.00827	0.104	0.557
kag_000_14059	Co ₄ GaMn ₃	8	-7.014	-7.155	-2.000e-06	0.00458	0.199	0.188
kag_000_14079	Ni ₆ PtSn	8	-5.187	-5.45	0.000e+00	0.00341	0.347	0.293
kag_000_14092	AsCl ₅ Tb ₃ W	10	-4.099	-5.107	-3.000e-06	0.00506	1.584	3.081
kag_000_14095	EuNi ₃ Pt ₄ Sn ₃	11	-4.79	-5.231	-5.000e-06	0.0068	1.034	0.917
kag_000_14115	Co ₈ Zr ₄	12	-7.747	-7.837	-4.000e-05	0.0094	0.371	0.412
kag_000_14117	Al ₂ AsGaRu ₃ U	8	-6.864	-7.073	-2.000e-06	0.00743	0.91	2.088
kag_000_14131	AlEu ₂ GaGd ₃ Nd	8	-3.615	-3.781	0.000e+00	0.0047	2.072	2.683
kag_000_14133	GaKPbTl ₂ Yb ₃	8	-1.99	-2.368	-3.000e-06	0.00451	2.508	2.707
kag_000_14141	AlCo ₄ LaPr	7	-5.433	-5.968	-6.000e-06	0.00825	0.603	1.638
kag_000_14161	Dy ₄ EuSnYb ₂	8	-3.373	-3.46	-3.000e-06	0.00332	1.259	1.856
kag_000_14164	Na ₅ Yb ₃	8	-1.28	-1.286	0.000e+00	0.00282	0.331	0.163
kag_000_14215	NbNi ₁₁	12	-5.855	-5.923	3.000e-06	0.00758	0.304	0.398
kag_000_14224	K ₂ Na ₂ TlYb ₃	8	-1.278	-1.354	-5.000e-06	0.00332	1.215	1.099
kag_000_14230	Fe ₅ Pt ₂ Zn	8	-6.587	-6.621	2.000e-06	0.00884	0.111	0.153
kag_000_14258	Pt ₅ Ru ₃	8	-6.989	-7.205	2.000e-06	0.00312	0.43	0.958
kag_000_14269	Cs ₃ KTb ₃	7	-1.815	-1.938	-1.000e-06	0.00195	0.989	0.919
kag_000_14291	LuPd ₄ Ru ₃	8	-6.724	-6.754	0.000e+00	0.00411	0.148	0.129
kag_000_14303	Fe ₅ PdRhTi	8	-7.479	-7.593	-2.000e-06	0.00518	0.353	2.184
kag_000_14308	Er ₂ Fe ₃ MgP ₄	10	-5.634	-6.365	-6.000e-06	0.00526	1.391	1.463
kag_000_14324	Na ₅ Nd ₃	8	-2.289	-2.332	-1.000e-06	0.00306	0.662	0.375
kag_000_14357	Ni ₈	8	-5.376	-5.41	-5.100e-05	0.00642	0.217	0.204
kag_000_14433	AlCoNi ₆	8	-5.507	-5.591	0.000e+00	0.00372	0.433	0.228
kag_000_14436	CoDy ₃ S ₅ TaTi ₂	12	-5.844	-6.734	-1.000e-06	0.00454	1.489	2.599
kag_000_14477	AlNi ₇	8	-5.427	-5.445	-1.000e-05	0.00421	0.209	0.108
kag_000_14489	PdPt ₄ Ru ₃	8	-6.685	-7.074	-3.000e-06	0.00688	0.788	1.158
kag_000_14492	Br ₂ Nd ₃ Sn ₂ Tl	8	-3.458	-4.146	-1.000e-06	0.00708	0.81	3.747
kag_000_14578	Ba ₃ Nd ₃ SbSn ₄ Tl	12	-3.664	-3.835	-4.000e-06	0.00573	0.31	1.926

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_14579	As ₂ Fe ₃ Mn ₂ Si	8	-7.003	-7.135	3.000e-06	0.00561	0.451	0.429
kag_000_14581	Fe ₅ Mg ₄ Ni ₃	12	-5.215	-5.285	1.200e-05	0.00911	0.17	0.128
kag_000_14582	CaDy ₃ Eu ₂ Mg ₂	8	-2.672	-2.739	0.000e+00	0.00298	1.656	3.106
kag_000_14588	Co ₇ Ge	8	-6.456	-6.639	-1.200e-05	0.00794	0.707	0.383
kag_000_14612	DyMn ₄ Pt ₃	8	-6.932	-7.304	0.000e+00	0.00883	0.536	1.613
kag_000_14613	Cd ₃ Ga ₄ Li ₂ Nd ₃	12	-2.646	-2.949	-5.000e-06	0.00524	1.315	2.043
kag_000_14652	Na ₃ Tb ₃ Tl ₂	8	-2.433	-2.755	-1.000e-06	0.00465	2.3	2.261
kag_000_14655	Ba ₂ EuInSrYb ₃	8	-1.79	-1.832	-4.000e-06	0.00317	0.7	1.481
kag_000_14656	AlFe ₃ Mn ₃ Pt	8	-7.51	-7.665	1.000e-06	0.0063	0.33	2.15
kag_000_14657	K ₅ Nd ₃	8	-1.896	-1.934	-1.000e-06	0.00368	0.861	1.018
kag_000_14659	Cr ₄ S ₅ Tb ₃	12	-5.778	-6.796	5.000e-06	0.00541	1.026	2.631
kag_000_14677	Ni ₈	8	-5.335	-5.411	2.000e-06	0.00344	0.388	0.291
kag_000_14699	Co ₃ Cr ₂ Ni ₃	8	-6.749	-6.98	-1.100e-05	0.00757	0.103	0.28
kag_000_14700	Ce ₂ Dy ₃ Tl ₃	8	-4.129	-4.205	2.000e-06	0.00531	0.312	1.05
kag_000_14702	Dy ₃ EuIn ₃ Sb	8	-3.692	-3.857	0.000e+00	0.0036	0.437	1.067
kag_000_14710	Eu ₅ Tb ₃	8	-2.686	-2.746	-3.200e-05	0.00387	0.405	1.142
kag_000_14775	GeMn ₃ Zr ₃	7	-7.947	-8.279	0.000e+00	0.00472	0.727	0.97
kag_000_14794	GaNbNi ₄ U	7	-6.534	-6.752	-1.100e-05	0.00804	0.228	0.587
kag_000_14805	Al ₂ Br ₅ Gd ₃	10	-3.154	-3.911	-9.000e-06	0.00638	1.058	3.441
kag_000_14808	AlCo ₇	8	-6.445	-6.617	-4.000e-06	0.00463	0.433	0.239
kag_000_14825	Ge ₃ Ru ₃ S ₄ Tl ₂	12	-4.935	-5.294	-1.000e-06	0.00801	0.914	1.92
kag_000_14828	Al ₈ FeMn ₃	12	-5.314	-5.497	-8.000e-06	0.0063	0.645	1.353
kag_000_14848	Ru ₅ SnZr	7	-8.004	-8.31	-5.000e-06	0.00627	0.519	1.449
kag_000_14850	Pt ₃ Ru ₄	7	-7.296	-7.597	-1.000e-06	0.00646	0.685	0.499
kag_000_14906	CrPtRu ₃ Y ₃	8	-7.104	-7.942	-1.100e-05	0.00622	0.869	2.556
kag_000_14913	Dy ₃ GaGeMn ₃	8	-5.069	-6.044	-6.000e-06	0.00745	0.908	2.571
kag_000_14951	Dy ₃ EuIn ₂ Na ₂	8	-2.895	-3.032	0.000e+00	0.00594	1.007	0.766
kag_000_14963	Al ₂ Ce ₂ CoFe ₃	8	-5.683	-6.607	-1.050e-04	0.00999	1.185	1.562
kag_000_14971	Fe ₃ La ₂ Si ₃	8	-6.45	-6.62	-2.000e-06	0.00748	0.348	0.387
kag_000_15000	Mn ₄ PPtSi ₃	9	-6.346	-7.161	-6.000e-05	0.00548	0.894	2.832
kag_000_15016	Al ₄ Fe ₃	7	-5.412	-5.809	1.000e-05	0.00506	0.724	0.837
kag_000_15070	Br ₃ IKTb ₃	8	-2.866	-3.526	-1.000e-06	0.00539	2.273	5.168
kag_000_15087	Co ₃ Pt ₅	8	-6.083	-6.324	-8.000e-06	0.00354	0.223	0.779
kag_000_15105	Al ₂ Co ₂ Fe ₄	8	-6.618	-6.814	5.000e-06	0.00664	0.307	0.909
kag_000_15113	Dy ₃ Na ₂ Sn ₂	7	-3.509	-3.511	2.000e-06	0.00845	0.385	0.252
kag_000_15120	HCo ₃ Fe ₃ Ga	8	-5.961	-6.241	1.300e-05	0.00626	0.45	2.274
kag_000_15122	Gd ₄ Na ₄	8	-2.629	-2.642	-2.000e-06	0.00165	0.169	0.219
kag_000_15141	CoFe ₅ Ni ₂	8	-6.847	-7.195	-5.000e-06	0.00426	0.711	1.095
kag_000_15194	KSe ₂ Tb ₃	6	-3.416	-4.409	7.000e-06	0.00469	1.393	3.767
kag_000_15200	Al ₃ BaNi ₂ Tb ₄	10	-4.215	-4.485	6.000e-06	0.00874	0.642	2.669
kag_000_15203	CeDy ₃ EuIn ₂	7	-4.601	-3.934	-5.000e-06	0.00486	1.079	2.646
kag_000_15243	Ru ₄ Se ₆ Sn	11	-4.843	-5.641	1.000e-06	0.00403	0.576	1.965
kag_000_15273	BaInPbYb ₅	8	-2.253	-2.189	-3.000e-05	0.00991	1.794	2.564
kag_000_15280	Co ₂ Gd ₃ I ₄ Sn ₂	11	-3.558	-4.249	-1.000e-06	0.00926	1.491	3.848
kag_000_15337	Dy ₃ EuGaLa ₂ Sn	8	-4.083	-4.308	-4.000e-06	0.00446	1.9	2.822
kag_000_15364	Ce ₂ Dy ₃ NaPbTl	8	-4.021	-4.199	-5.000e-06	0.00761	2.119	2.746
kag_000_15372	FeMn ₃ P ₈	12	-5.97	-6.677	-1.000e-06	0.00687	0.842	1.589
kag_000_15379	Eu ₂ LaPb ₂ Tb ₃	8	-3.727	-3.867	0.000e+00	0.00388	0.977	1.41
kag_000_15396	EuGd ₅ Pt ₂	8	-4.71	-5.187	-2.000e-06	0.00472	1.037	1.036
kag_000_15407	AlFe ₄ Pt ₃	8	-6.81	-6.946	-3.000e-06	0.00548	0.394	1.403
kag_000_15417	BrCo ₂ CrGd ₃ MnS ₄	12	-5.294	-6.088	-7.000e-06	0.00897	0.501	2.853
kag_000_15420	BaKSn ₂ Tb ₃	7	-3.234	-3.698	0.000e+00	0.0052	2.22	2.628

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_15430	Ba ₂ Gd ₄ Sn ₂	8	-3.729	-3.925	-6.000e-06	0.00339	1.777	2.624
kag_000_15440	MgPtRu ₃ SnTm	7	-6.19	-6.42	-1.000e-06	0.00379	0.336	0.351
kag_000_15449	Lu ₄ Ru ₃ Y	8	-6.281	-6.612	-2.000e-06	0.00822	1.242	2.361
kag_000_15453	AgFe ₃ Pd ₂ Sn ₃	9	-5.114	-5.321	2.000e-06	0.00421	0.649	0.451
kag_000_15458	FeNi ₄ PdPtSn	8	-5.141	-5.597	7.000e-06	0.0058	0.623	1.417
kag_000_15481	Cs ₃ Yb ₃	6	-0.871	-0.887	-1.250e-05	0.00362	0.315	0.244
kag_000_15489	Co ₆ GeTi	8	-6.866	-6.913	-6.000e-06	0.00506	0.174	0.104
kag_000_15533	Ba ₃ Nd ₃ Pb	7	-3.128	-3.355	-2.000e-06	0.00362	0.899	3.353
kag_000_15565	AlGaMn ₃ Rh ₂ Si	8	-6.681	-6.851	-1.000e-06	0.00707	0.312	0.321
kag_000_15571	Dy ₃ GdLa ₂ Sn ₂	8	-4.643	-4.727	0.000e+00	0.00887	0.525	1.164
kag_000_15589	Fe ₆ Pt ₂	8	-7.22	-7.516	0.000e+00	0.00655	0.71	0.896
kag_000_15597	Br ₄ ClGd ₃ Ir	9	-3.544	-4.907	-4.000e-06	0.00401	1.407	2.224
kag_000_15608	AlCoInaNi ₂ SnSrTb ₃	11	-3.913	-4.233	-6.000e-06	0.00466	1.64	3.541
kag_000_15620	Ce ₂ Ni ₄	6	-5.878	-5.996	-2.000e-06	0.00417	0.2	0.974
kag_000_15642	Br ₅ CoTb ₃	9	-3.722	-4.178	-1.000e-06	0.00786	1.488	1.183
kag_000_15662	Dy ₃ Tl ₅	8	-2.878	-3.308	-1.000e-06	0.00214	0.797	0.536
kag_000_15673	Fe ₃ Ga ₃ LaSm	8	-4.779	-5.429	0.000e+00	0.00378	1.147	2.792
kag_000_15744	AlGd ₃ Sr ₃ Zn	8	-2.738	-2.952	0.000e+00	0.00454	0.992	4.28
kag_000_15753	Cs ₃ KYb ₃	7	-0.921	-0.965	-3.400e-06	0.00438	0.606	0.401
kag_000_15764	CoRu ₆ Zr	8	-8.662	-8.792	-1.700e-05	0.00609	0.257	0.88
kag_000_15799	Te ₂ Tl ₂ Yb ₃	7	-2.384	-2.92	1.000e-06	0.00252	2.063	1.634
kag_000_15819	Pt ₅ Ru ₃	8	-7.113	-7.202	-4.000e-06	0.00469	0.266	0.16
kag_000_15829	Dy ₃ SbTl ₄	8	-3.439	-3.63	-1.000e-06	0.00312	1.52	2.628
kag_000_15850	Dy ₄ GaLaSnSr	8	-3.998	-4.113	0.000e+00	0.00733	1.331	1.044
kag_000_15864	Ce ₂ Dy ₃ Tl ₃	8	-4.004	-4.207	-3.900e-05	0.00946	0.574	1.246
kag_000_15881	Al ₃ Ni ₅	8	-5.146	-5.35	3.000e-06	0.00536	0.697	0.418
kag_000_15891	FeNi ₈ Y	10	-5.759	-5.898	-1.000e-06	0.00665	0.222	0.481
kag_000_15900	Dy ₃ Na ₄ Tl	8	-2.355	-2.462	0.000e+00	0.00728	0.546	0.395
kag_000_15926	Dy ₃ Na ₅	8	-2.186	-2.217	0.000e+00	0.00517	0.625	0.541
kag_000_15948	BrI ₃ Tb ₃ Tl	8	-2.978	-3.515	-1.000e-06	0.00373	1.403	1.054
kag_000_15954	FeGe ₂ Ni ₅	8	-5.468	-5.701	-3.000e-06	0.00747	0.898	0.398
kag_000_15956	Fe ₄ GaPt ₃	8	-6.586	-6.682	-9.000e-06	0.006	0.25	0.841
kag_000_15975	CoHoNi ₆ Si ₂	10	-5.763	-5.938	-3.400e-05	0.00943	1.127	1.018
kag_000_15983	Na ₂ SnTb ₃ Tl ₂	8	-3.095	-3.21	-1.000e-06	0.00427	1.126	2.553
kag_000_15991	Cs ₄ Gd ₃	7	-1.883	-1.896	-5.000e-06	0.00353	0.249	0.218
kag_000_15996	Co ₃ Fe ₃ NbPt	8	-7.68	-7.695	-8.000e-06	0.00561	0.094	0.133
kag_000_16025	EuKNaNd ₃ Sr ₂	8	-2.395	-2.42	-3.000e-06	0.00374	0.312	0.328
kag_000_16037	HgNa ₂ Pb ₂ Tb ₃	8	-2.985	-3.041	-4.000e-06	0.00407	0.277	0.21
kag_000_16040	Co ₅ GeSi	7	-6.183	-6.45	-1.000e-06	0.0081	1.134	1.811
kag_000_16042	Co ₄ GeNi ₃	8	-5.952	-6.098	1.000e-06	0.00279	0.607	0.9
kag_000_16044	Ru ₅ TbU	7	-8.43	-8.954	-2.000e-06	0.0063	0.427	1.334
kag_000_16045	Dy ₃ Na ₅	8	-2.159	-2.212	2.000e-06	0.00434	0.234	1.26
kag_000_16046	Co ₅ Ni ₂ Pt	8	-6.17	-6.35	-8.400e-05	0.00757	0.706	0.889
kag_000_16086	Co ₈	8	-6.729	-6.841	-4.400e-05	0.00838	0.304	0.182
kag_000_16123	Ni ₅ Ru ₃ ScY ₃	12	-7.024	-7.082	-4.400e-05	0.00796	0.17	0.147
kag_000_16130	GeMn ₄ Pt ₃	8	-6.907	-7.313	-1.000e-05	0.00844	0.708	1.667
kag_000_16146	Ni ₃ Zr ₇	10	-7.733	-7.803	1.000e-06	0.00837	0.104	0.17
kag_000_16151	H ₂ Fe ₃ Pt ₄	9	-5.886	-6.003	-3.000e-06	0.00663	0.338	1.325
kag_000_16202	Al ₃ GaMn ₄	8	-6.021	-6.281	-2.900e-05	0.00596	0.382	0.458
kag_000_16258	Na ₅ Tb ₃	8	-2.186	-2.236	1.000e-06	0.00237	0.62	1.101
kag_000_16269	CoPt ₃ Ru ₃	7	-7.229	-7.29	-1.000e-06	0.00826	0.168	0.171
kag_000_16290	Nd ₂ Ni ₄	6	-5.493	-5.526	0.000e+00	0.00713	0.186	0.16

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_16295	Gd ₃ PdSe ₄ SiSn	10	-4.549	-5.307	-2.000e-06	0.0063	2.572	2.497
kag_000_16308	Mn ₅ PdPtSn	8	-7.18	-7.276	0.000e+00	0.0039	0.213	0.31
kag_000_16315	Cl ₂ INd ₃ SiTe ₂	9	-3.784	-4.552	0.000e+00	0.00484	1.638	2.972
kag_000_16316	AlFe ₄ GaMnSn	8	-6.211	-6.294	-3.600e-05	0.00532	0.265	2.746
kag_000_16352	GePt ₃ Ru ₄	8	-6.877	-7.427	1.000e-06	0.0067	0.765	2.433
kag_000_16357	AgMn ₃ RuSn ₂	7	-5.912	-6.189	0.000e+00	0.00394	0.849	1.224
kag_000_16389	Ga ₄ LaMgNi ₆	12	-4.521	-4.587	-1.600e-05	0.00657	0.226	0.187
kag_000_16395	Ho ₂ Ru ₄	6	-7.93	-7.96	-9.000e-06	0.00493	0.127	0.052
kag_000_16405	Cl ₂ IrK ₂ Sn ₂ Tb ₃	10	-3.586	-4.472	-2.000e-06	0.00522	2.531	3.635
kag_000_16419	EuGa ₂ Nd ₅	8	-3.947	-4.13	-1.200e-05	0.00989	2.038	1.279
kag_000_16430	I ₅ RhYb ₃	9	-2.709	-3.281	-3.000e-06	0.00574	1.212	3.066
kag_000_16432	GaNiPt ₂ Ru ₄	8	-7.096	-7.162	-1.000e-06	0.00488	0.12	1.431
kag_000_16440	GaNd ₂ Ni ₃	6	-4.517	-5.101	1.300e-05	0.00676	1.141	1.115
kag_000_16441	Na ₄ Tb ₃ Tl	8	-2.38	-2.478	-4.000e-06	0.00337	0.454	3.229
kag_000_16456	Cs ₅ Tb ₃	8	-1.503	-1.721	-4.000e-06	0.00203	1.379	2.113
kag_000_16474	Fe ₂ Mn ₈ Si ₂	12	-8.192	-8.385	-2.000e-05	0.0062	0.62	0.691
kag_000_16486	NaSr ₄ Tb ₃	8	-2.287	-2.444	2.000e-06	0.00285	0.542	0.386
kag_000_16507	Nd ₃ Tl ₅	8	-3.185	-3.387	0.000e+00	0.00173	0.834	0.413
kag_000_16546	Sb ₅ Tb ₃	8	-4.359	-4.94	0.000e+00	0.00377	1.705	1.623
kag_000_16557	Cu ₅ Fe ₃ Gd ₄	12	-5.18	-5.198	-4.900e-05	0.00626	0.122	0.137
kag_000_16581	Mn ₃ NiSn ₈	12	-3.982	-5.034	5.000e-06	0.00836	0.929	1.587
kag_000_16584	Co ₂ Fe ₃ Ni ₅ Zr	11	-6.497	-6.646	-1.590e-04	0.00871	0.278	0.382
kag_000_16643	Ni ₄ Pt ₃ Si	8	-5.848	-5.938	-6.000e-06	0.00794	0.278	0.196
kag_000_16644	Co ₃ ErScSnTi	7	-6.096	-6.475	-4.000e-06	0.00504	0.308	1.353
kag_000_16646	AlCo ₇	8	-6.594	-6.616	5.000e-06	0.00652	0.089	0.074
kag_000_16652	Ga ₃ Ni ₄ V	8	-5.039	-5.167	5.000e-06	0.00622	0.598	0.529
kag_000_16653	Br ₈ Mn ₄	12	-4.054	-4.216	2.000e-05	0.0072	0.655	0.549
kag_000_16655	Cl ₃ CsGd ₃ Pt	8	-3.593	-4.438	3.000e-06	0.00379	1.478	3.801
kag_000_16673	Na ₂ SrTb ₃ Tl	7	-2.531	-2.757	-1.000e-06	0.00561	1.96	4.416
kag_000_16712	EuKNaSrYb ₄	8	-1.326	-1.358	-2.000e-06	0.00353	0.603	0.275
kag_000_16713	Ga ₂ MgNi ₃ Y	7	-4.391	-4.655	-1.300e-05	0.00841	0.45	0.705
kag_000_16740	AlMn ₄ PdSnTi	8	-6.791	-7.033	-3.301e-02	0.00639	0.925	3.015
kag_000_16763	AlFe ₄ GaY	7	-6.174	-6.584	-5.000e-06	0.00792	0.537	0.603
kag_000_16768	Na ₅ Nd ₃	8	-2.305	-2.331	-1.000e-06	0.00425	0.636	0.281
kag_000_16771	Gd ₃ I ₅ SiSn	10	-2.661	-3.899	-2.000e-06	0.00826	1.769	3.099
kag_000_16772	KNa ₃ SnYb ₃	8	-1.457	-1.668	-7.000e-06	0.00309	2.006	3.965
kag_000_16790	NiPt ₂ Ru ₄	7	-7.408	-7.54	-2.000e-06	0.00678	0.641	0.526
kag_000_16809	Ga ₂ Pt ₂ Ru ₄	8	-6.74	-6.979	1.000e-06	0.00449	0.686	0.367
kag_000_16813	CoFe ₃ Tm ₂	6	-6.763	-6.839	-2.000e-06	0.00549	0.273	0.169
kag_000_16871	Ga ₃ MgNi ₄	8	-4.103	-4.21	1.000e-06	0.00703	0.554	1.413
kag_000_16890	Co ₃ Mn ₃ Ni ₂	8	-7.046	-7.247	-2.500e-05	0.00894	0.244	0.114
kag_000_16909	Cs ₄ Yb ₃	7	-0.918	-0.931	1.000e-07	0.00091	0.38	0.43
kag_000_16916	Gd ₃ KNa ₃ Yb	8	-2.198	-2.23	0.000e+00	0.00382	0.397	0.226
kag_000_16942	BaNa ₄ Tb ₃	8	-2.263	-2.304	-4.000e-06	0.00166	0.525	0.48
kag_000_16952	Al ₂ Gd ₄ Lu ₂	8	-4.234	-4.529	-1.000e-06	0.00558	1.743	2.436
kag_000_16971	Fe ₄ Si ₅ Zr	10	-6.927	-7.241	-1.600e-05	0.00822	0.449	0.49
kag_000_16977	Al ₂ GaPtRu ₃ U	8	-6.827	-7.34	2.000e-06	0.0043	1.05	1.94
kag_000_17042	Co ₃ Fe ₄ Ni ₅	12	-6.487	-6.604	0.000e+00	0.00608	0.23	0.264
kag_000_17043	Br ₃ Gd ₃ K ₂ Mn ₂	10	-3.45	-4.103	-4.000e-06	0.00942	1.195	2.066
kag_000_17063	Cl ₂ Gd ₃ KRb ₂ Si ₂	10	-2.862	-3.723	-2.000e-06	0.00597	1.791	3.541
kag_000_17064	GaGeHfMn ₄	7	-7.234	-7.693	2.400e-05	0.00731	0.454	0.454
kag_000_17069	KNaTl ₂ Yb ₄	8	-1.569	-1.659	8.000e-06	0.00445	1.807	3.156

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_17107	Na ₅ Tb ₃	8	-2.173	-2.231	-4.000e-06	0.00341	0.418	0.359
kag_000_17110	RhSe ₄ Tb ₃ Tl	9	-4.562	-5.323	0.000e+00	0.00361	0.999	2.697
kag_000_17124	AlCo ₇	8	-6.552	-6.617	-1.000e-05	0.00424	0.136	0.117
kag_000_17147	Dy ₄ In ₂ LuSn	8	-4.081	-4.333	0.000e+00	0.00733	0.807	0.404
kag_000_17156	Dy ₃ Na ₅	8	-2.191	-2.217	-2.000e-06	0.00158	0.582	0.337
kag_000_17164	Fe ₅ Pt ₃	8	-7.098	-7.292	3.000e-06	0.00546	0.391	0.251
kag_000_17170	Ni ₄ Tm ₂	6	-5.626	-5.63	1.000e-06	0.00743	0.062	0.046
kag_000_17176	Co ₁₀ Ga ₂	12	-6.24	-6.287	-1.400e-05	0.00918	0.199	0.276
kag_000_17182	PtSn ₂ Tb ₄ Tl	8	-4.553	-4.854	-5.000e-06	0.00313	0.861	1.704
kag_000_17192	Ga ₂ Nb ₂ SeTe ₄ Yb ₃	12	-3.879	-4.604	-4.000e-06	0.00602	1.276	4.131
kag_000_17199	Co ₄ Ga ₂ Pr	7	-5.234	-5.621	-3.700e-05	0.0053	0.543	0.81
kag_000_17234	AlGeMn ₄ NiOs	8	-7.435	-7.611	1.000e-06	0.00554	0.756	1.682
kag_000_17236	CaGd ₃ IRh ₃ SbSnTe	11	-4.819	-5.231	-1.000e-06	0.00517	1.331	2.653
kag_000_17240	Al ₃ Fe ₃ La ₂ Ru	9	-5.906	-6.184	2.000e-06	0.0078	0.874	1.062
kag_000_17272	CaGdP ₃ Ru ₃	8	-6.415	-6.767	-2.000e-06	0.00598	0.849	0.436
kag_000_17286	Ni ₄ Y ₂	6	-6.158	-6.223	-4.400e-05	0.00749	0.21	1.022
kag_000_17294	Mn ₃ Pt ₅	8	-6.962	-7.108	8.000e-06	0.00909	0.299	1.469
kag_000_17308	Ce ₂ Mn ₃ PdRh ₃	9	-7.409	-7.537	3.000e-06	0.00867	0.255	0.269
kag_000_17332	AuGe ₂ La ₂ Ni ₃ PtZn	10	-4.337	-5.043	-5.000e-06	0.00665	1.449	1.911
kag_000_17342	LaRb ₂ Tb ₃ Tl ₂	8	-2.674	-2.994	-1.300e-05	0.00501	1.633	3.202
kag_000_17348	Co ₇ Fe	8	-6.858	-6.992	-3.000e-06	0.00598	0.329	0.202
kag_000_17385	Eu ₅ Yb ₃	8	-1.51	-1.706	-1.000e-06	0.00187	1.36	0.783
kag_000_17397	Ca ₃ Gd ₅	8	-3.401	-3.48	1.000e-06	0.00189	1.036	0.538
kag_000_17411	Dy ₃ La ₂ NaTl ₂	8	-3.521	-3.749	0.000e+00	0.00955	2.05	1.203
kag_000_17418	Au ₂ CeRu ₃ Sn	7	-5.974	-6.285	-6.000e-06	0.00702	0.458	0.536
kag_000_17425	Al ₂ Fe ₈ Ti ₂	12	-7.233	-7.357	-3.000e-06	0.00519	0.373	0.451
kag_000_17436	Ga ₃ Gd ₃ TlTm	8	-3.728	-4.046	-2.000e-06	0.00909	1.183	2.419
kag_000_17478	Lu ₇ Ni ₅	12	-5.074	-5.149	-2.000e-06	0.00985	0.443	0.365
kag_000_17526	Dy ₇ Sn	8	-4.68	-4.611	-2.000e-06	0.00318	0.265	0.207
kag_000_17528	Fe ₄ Ga ₃ SiTb ₄	12	-5.425	-5.698	0.000e+00	0.00424	0.643	0.745
kag_000_17553	Nd ₃ Sn ₉	12	-4.186	-4.301	-3.000e-06	0.00692	0.515	2.619
kag_000_17587	AlNi ₇	8	-5.38	-5.444	-8.000e-06	0.0054	0.53	0.362
kag_000_17601	EuGd ₃ MgSn ₂ Sr	8	-3.496	-3.668	-3.000e-06	0.00781	0.684	1.356
kag_000_17619	AgSn ₂ Tb ₄ Tl	8	-3.898	-4.252	0.000e+00	0.00446	1.319	0.842
kag_000_17631	Gd ₃ Na ₂ Te ₂ Tl	8	-3.261	-3.584	0.000e+00	0.00379	1.501	1.586
kag_000_17685	CoMn ₄ Pt ₂ Ti	8	-7.799	-8.03	-1.000e-05	0.00918	0.486	1.562
kag_000_17699	Ce ₂ GeRu ₄	7	-7.549	-7.9	1.000e-06	0.00943	0.963	1.695
kag_000_17708	CdNi ₄ SiZn	7	-4.021	-4.206	-7.000e-06	0.00921	0.606	2.868
kag_000_17711	AuFe ₄ Hf ₂	7	-7.68	-8.047	-2.100e-05	0.00565	0.538	1.966
kag_000_17718	Gd ₄ InTl ₃	8	-3.611	-3.732	0.000e+00	0.00675	0.616	0.386
kag_000_17738	EuLaNd ₃ PbSbZn	8	-3.919	-4.1	-5.000e-06	0.00477	2.24	3.462
kag_000_17805	Lu ₅ Nd ₃	8	-4.48	-4.521	-2.000e-06	0.00102	0.263	0.173
kag_000_17840	La ₂ Ru ₄	6	-6.856	-7.38	0.000e+00	0.00693	0.693	1.209
kag_000_17853	Eu ₂ Gd ₃ HgNa ₂	8	-2.38	-2.511	-3.700e-05	0.00644	1.596	1.167
kag_000_17882	InNa ₄ Yb ₃	8	-1.675	-1.514	-3.000e-06	0.00354	1.465	1.916
kag_000_17900	Ni ₈	8	-5.304	-5.414	8.000e-06	0.0051	0.205	0.174
kag_000_17916	Na ₅ Tb ₃	8	-2.193	-2.233	1.000e-06	0.00478	0.469	0.344
kag_000_17929	GeNi ₅ PtTc	8	-5.906	-6.105	-7.000e-06	0.00836	0.715	1.107
kag_000_17944	Na ₅ Tb ₃	8	-2.158	-2.236	0.000e+00	0.00437	0.956	1.27
kag_000_17953	FeLiMn ₃ NiPtSb	8	-6.272	-6.456	0.000e+00	0.00579	1.232	2.031
kag_000_17955	Gd ₃ Se ₂ SmTe ₂	8	-4.479	-5.397	0.000e+00	0.00488	1.204	2.493
kag_000_17964	CdGd ₃ K ₂ Sr ₂	8	-2.103	-2.198	1.000e-06	0.00325	1.094	1.137

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_17991	Ga ₂ MgNi ₅	8	-4.475	-4.622	-1.000e-06	0.00726	0.827	1.793
kag_000_18010	Pt ₅ Ru ₃	8	-7.088	-7.195	-4.000e-06	0.00445	0.16	0.12
kag_000_18024	CrDy ₃ GaSe ₅ Ti ₂	12	-4.974	-5.844	-2.000e-06	0.00377	1.924	4.92
kag_000_18030	Co ₄ Ni ₄	8	-5.946	-6.074	-3.000e-05	0.00928	0.677	0.3
kag_000_18031	Eu ₃ Tl ₂ Yb ₃	8	-1.835	-2.069	2.000e-06	0.00609	1.895	1.968
kag_000_18040	AlCo ₅ FeNi	8	-6.546	-6.555	1.000e-06	0.00858	0.058	1.274
kag_000_18061	Ni ₈	8	-5.36	-5.411	-1.100e-05	0.00093	0.257	0.775
kag_000_18077	Br ₅ CuGaIrNd ₃	11	-3.511	-4.382	-5.000e-06	0.00481	1.874	3.273
kag_000_18087	AuGa ₂ Ni ₃ Zr	7	-4.906	-5.235	0.0000e+00	0.00588	0.64	0.66
kag_000_18097	AsCo ₃ GePt ₃	8	-5.828	-6.057	-9.000e-06	0.00912	0.264	0.936
kag_000_18101	Co ₃ PdPt ₄	8	-6.184	-6.203	-4.000e-06	0.0053	0.127	0.136
kag_000_18104	Ni ₆ Si ₂	8	-5.765	-5.922	-8.000e-06	0.00588	0.45	0.335
kag_000_18134	AgEuNa ₂ Yb ₃	7	-1.441	-1.669	-2.000e-06	0.01	1.224	2.756
kag_000_18148	Co ₃ CrNi ₄	8	-6.394	-6.44	1.000e-06	0.0059	0.255	0.137
kag_000_18149	Al ₃ CoFe ₆ GdMg	12	-5.872	-6.153	-2.000e-06	0.00858	0.378	1.177
kag_000_18151	Ba ₃ Si ₆ Tb ₃	12	-4.206	-4.655	-8.000e-06	0.00411	1.421	1.449
kag_000_18157	Ca ₂ K ₂ NaYb ₃	8	-1.265	-1.305	-2.000e-06	0.00723	1.072	2.465
kag_000_18196	Fe ₅ GdSn	7	-6.461	-6.836	-1.600e-05	0.00541	0.373	0.565
kag_000_18212	I ₂ Nd ₃ S ₃ Si ₂	10	-4.165	-4.823	0.0000e+00	0.00629	1.793	2.204
kag_000_18225	Fe ₈ Lu ₄	12	-6.97	-7.02	3.000e-06	0.00745	0.156	0.104
kag_000_18240	Na ₃ Tb ₃ Tl ₂	8	-2.542	-2.742	1.000e-06	0.00363	1.971	3.282
kag_000_18263	CaDy ₃ Tl ₃	7	-2.94	-3.411	-1.000e-06	0.00282	2.498	1.502
kag_000_18276	Dy ₂ Ru ₄	6	-7.407	-7.904	0.0000e+00	0.00795	0.876	0.606
kag_000_18286	CaGa ₂ Nd ₃ Yb	7	-3.174	-3.518	-3.000e-06	0.00441	1.85	3.397
kag_000_18303	CoNi ₇	8	-5.467	-5.57	-1.000e-06	0.00295	0.36	0.857
kag_000_18307	Dy ₃ Eu ₃ Ga ₆	12	-3.158	-3.509	4.000e-06	0.00919	1.074	1.025
kag_000_18359	Ni ₆ Pt ₂	8	-5.581	-5.631	-2.000e-06	0.00378	0.18	0.148
kag_000_18408	Ge ₂ Ni ₆	8	-5.332	-5.396	3.000e-06	0.00373	0.41	0.349
kag_000_18413	GaLaNbRu ₃ Si ₂	8	-6.896	-7.29	-2.000e-06	0.00907	1.432	3.472
kag_000_18416	Br ₅ Nd ₃ Sn ₂ Ta	11	-3.605	-4.612	-1.000e-06	0.00413	1.904	3.506
kag_000_18421	Co ₇ Pt	8	-6.521	-6.728	-4.000e-06	0.00673	0.677	1.147
kag_000_18442	AlGaGeNi ₄ PSc ₂	10	-5.471	-5.6	-3.000e-06	0.00906	0.363	0.368
kag_000_18461	CaEuNa ₃ Tb ₃	8	-2.377	-2.417	2.000e-06	0.00195	0.613	1.201
kag_000_18473	Dy ₄ Mg ₂ Sn ₅	11	-3.778	-3.958	-4.000e-05	0.00761	1.164	0.795
kag_000_18482	Pt ₄ Ru ₄	8	-7.324	-7.588	-4.000e-06	0.00449	0.603	0.409
kag_000_18486	Co ₃ GeNiY ₃	8	-6.324	-6.563	-3.300e-05	0.00836	0.634	0.727
kag_000_18493	CaS ₇ Tb ₃	11	-4.999	-5.735	4.000e-06	0.00385	1.535	2.58
kag_000_18500	Na ₅ Nd ₃	8	-2.327	-2.329	-1.000e-06	0.00351	0.172	0.123
kag_000_18516	LuTb ₃ Tl ₄	8	-3.508	-3.593	-8.000e-06	0.00628	0.37	0.288
kag_000_18525	AlGa ₂ Ru ₃ Y	7	-6.19	-6.583	-4.000e-06	0.00225	0.297	0.574
kag_000_18528	NiPt ₃ Ru ₃ Zn	8	-6.321	-6.597	-1.000e-05	0.00863	0.434	0.389
kag_000_18549	Fe ₇ U	8	-8.48	-8.505	0.0000e+00	0.00244	0.174	1.331
kag_000_18556	AlGeMn ₃ Pt ₃	8	-6.487	-6.818	-3.800e-05	0.00796	0.274	0.331
kag_000_18557	BaDyNa ₃ Nd ₃	8	-2.74	-2.765	0.0000e+00	0.00434	0.963	1.673
kag_000_18559	Al ₂ Eu ₂ Fe ₃	7	-4.724	-5.063	0.0000e+00	0.00367	0.452	0.349
kag_000_18582	Pd ₄ S ₅ Tb ₃	12	-4.871	-5.686	-5.000e-06	0.00537	1.4	3.04
kag_000_18594	Eu ₂ Gd ₃ In ₂ Sn	8	-3.498	-3.643	0.0000e+00	0.00643	1.786	1.755
kag_000_18612	Al ₃ NiPtRu ₃	8	-6.496	-6.638	0.0000e+00	0.00616	0.364	0.903
kag_000_18636	Eu ₄ Gd ₃ Mg	8	-2.637	-2.744	-8.000e-06	0.00194	0.62	1.212
kag_000_18720	Ge ₂ Mn ₃ Pt ₂	7	-6.534	-6.747	-6.000e-06	0.00601	1.025	2.024
kag_000_18722	AlMnNi ₅ U	8	-6.34	-6.634	2.000e-06	0.00962	1.081	1.03
kag_000_18729	MgS ₈ Tb ₃	12	-4.606	-5.346	-1.000e-06	0.00477	1.955	3.021

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_18739	Pt ₄ Ru ₄	8	-7.478	-7.58	-6.000e-06	0.00664	0.218	0.183
kag_000_18761	Ni ₄ Pt ₂ Tb	7	-5.609	-5.855	1.500e-05	0.00887	0.908	1.332
kag_000_18762	Fe ₄ P ₆ Zr ₂	12	-6.886	-7.462	-1.200e-05	0.00842	0.838	0.965
kag_000_18786	Al ₂ Co ₅ CuHoSm	10	-5.415	-5.695	-5.000e-06	0.00812	0.769	0.647
kag_000_18794	Mn ₄ NiPt ₃	8	-7.386	-7.449	-2.700e-05	0.00604	0.151	0.83
kag_000_18816	GaHf ₂ Ru ₄	7	-8.454	-8.706	3.000e-06	0.00266	0.171	0.246
kag_000_18825	Ge ₃ La ₃ Ru ₃	9	-6.266	-6.548	-1.000e-06	0.00613	0.326	0.321
kag_000_18871	PbTl ₂ Yb ₅	8	-2.08	-2.291	-3.000e-06	0.00385	1.228	1.45
kag_000_18872	Br ₃ Cs ₂ Gd ₃ Sn ₂	10	-2.497	-3.645	-6.000e-06	0.0057	1.264	2.657
kag_000_18883	AlCrFe ₆	8	-7.631	-7.722	-1.000e-06	0.00596	0.141	0.756
kag_000_18904	Mn ₃ Pt ₅	8	-6.891	-7.105	-5.000e-06	0.00621	0.364	0.324
kag_000_18933	Gd ₅ GeNiTe ₂	9	-4.532	-5.034	-4.200e-05	0.0097	1.726	1.128
kag_000_18934	Be ₂ DyNi ₆ Np	10	-5.883	-5.945	-3.000e-06	0.00562	0.185	0.157
kag_000_18975	Ni ₇ Sn	8	-5.196	-5.286	-1.000e-06	0.00435	0.681	1.011
kag_000_18980	Ga ₃ Ni ₅	8	-4.652	-4.735	2.000e-06	0.00391	0.301	0.185
kag_000_18990	Mn ₄ Pt ₃ Re	8	-8.177	-8.33	1.000e-06	0.00769	0.34	0.905
kag_000_19026	BaSn ₂ Tl ₂ Yb ₃	8	-2.515	-2.699	4.000e-06	0.00254	0.617	0.401
kag_000_19042	AlCo ₄ Ni ₃	8	-6.041	-6.077	-2.000e-06	0.00449	0.162	0.145
kag_000_19058	Ho ₂ Ni ₄ Sn	7	-5.027	-5.302	-7.000e-06	0.00902	1.167	1.274
kag_000_19074	Co ₄ Dy ₂	6	-6.346	-6.384	-3.000e-06	0.00868	0.145	0.981
kag_000_19094	CoFe ₈ NiZn ₂	12	-6.295	-6.497	7.000e-06	0.00484	0.311	0.182
kag_000_19105	BrCaGd ₃ NaSnTl	8	-3.188	-3.495	0.000e+00	0.00518	1.096	1.179
kag_000_19139	BiBrLuPbTb ₃ Yb	8	-3.735	-4.078	0.000e+00	0.00952	1.748	1.433
kag_000_19144	GaGeMn ₄ Pt ₂	8	-6.614	-6.954	0.000e+00	0.00373	0.69	1.216
kag_000_19161	Co ₃ CuMn ₄	8	-7.197	-7.408	-2.980e-04	0.005	0.236	0.727
kag_000_19216	Cs ₂ Rb ₂ Yb ₃	7	-0.915	-0.963	5.600e-06	0.00131	0.656	0.58
kag_000_19220	Na ₂ Tl ₃ Yb ₃	8	-1.752	-1.918	-1.000e-06	0.00217	1.439	3.6
kag_000_19237	Se ₇ Tb ₃ Ti	11	-5.153	-5.522	0.000e+00	0.00345	0.903	2.002
kag_000_19241	Mn ₄ Pt ₃ Si	8	-7.172	-7.563	3.000e-06	0.00851	0.675	2.197
kag_000_19244	AlGeNi ₃ Si ₂ Ta ₃	10	-7.137	-7.347	-1.000e-06	0.00686	0.451	0.603
kag_000_19254	AlCoGd ₅ OSiSn	10	-5.245	-5.592	-4.000e-06	0.00815	0.745	1.425
kag_000_19269	Co ₄ Ga ₂ Pt ₂	8	-5.802	-5.85	-1.000e-06	0.00583	0.223	0.125
kag_000_19277	AlNi ₆ Zn	8	-4.922	-4.947	-1.300e-05	0.00426	0.27	0.729
kag_000_19290	Na ₃ Yb ₅	8	-1.292	-1.326	1.000e-06	0.00326	0.595	1.245
kag_000_19293	Ga ₂ Lu ₂ Tb ₄	8	-4.045	-4.364	-3.000e-06	0.00432	0.924	0.561
kag_000_19304	AgCsSbTe ₄ Yb ₃	10	-2.964	-3.39	-2.900e-05	0.00955	2.004	1.792
kag_000_19306	Gd ₃ Sr ₂ Tl ₃	8	-2.919	-3.147	1.000e-06	0.00355	0.928	2.223
kag_000_19312	AlCo ₃ Pt ₄	8	-5.762	-6.329	-1.700e-05	0.00721	0.45	0.33
kag_000_19315	Co ₅ Cr ₄ PtV ₂	12	-8.026	-8.06	2.000e-06	0.00687	0.149	0.189
kag_000_19331	Dy ₃ Na ₅	8	-2.176	-2.223	0.000e+00	0.00451	0.391	1.274
kag_000_19338	Ga ₂ LiNi ₃ Pt	7	-4.413	-4.665	-4.100e-05	0.00812	0.811	2.64
kag_000_19379	AlCo ₃ Ni ₄	8	-5.812	-5.916	-4.200e-05	0.00527	0.525	0.445
kag_000_19382	AlCoMn ₄	6	-6.984	-7.686	-1.800e-05	0.00761	0.513	0.69
kag_000_19384	Na ₅ Yb ₃	8	-1.265	-1.286	-9.000e-06	0.00308	0.82	0.549
kag_000_19392	Au ₂ Eu ₃ GeNi ₃ Sn	10	-3.554	-4.17	1.000e-06	0.00673	1.027	1.308
kag_000_19402	Dy ₃ Tl ₅	8	-2.902	-3.307	0.000e+00	0.00462	0.734	1.27
kag_000_19410	Cl ₄ IrTlYb ₃	9	-2.963	-4.119	0.000e+00	0.00402	2.383	5.77
kag_000_19415	CoGeRh ₂ Ru ₃ V	8	-7.62	-7.891	-1.000e-05	0.00765	0.618	1.123
kag_000_19425	Dy ₄ SnTl ₂	7	-3.732	-3.992	-1.000e-06	0.00531	0.618	0.439
kag_000_19429	AgCo ₄ Pt ₂ U	8	-6.299	-6.763	-5.600e-05	0.00969	1.077	1.8
kag_000_19472	Al ₉ Fe ₃	12	-4.798	-4.928	-4.100e-05	0.00696	0.337	0.359
kag_000_19489	BaInSbTb ₃ Tl	7	-3.712	-3.867	-1.000e-06	0.00368	1.239	2.69

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_19506	Co ₃ Ge ₄ Mn ₃ Tl	11	-5.915	-6.031	1.200e-05	0.00651	0.299	1.097
kag_000_19509	CeNd ₃ RbSn ₂	7	-3.892	-4.223	-1.000e-06	0.00795	1.807	0.951
kag_000_19557	Br ₄ ClNd ₃ Sn	9	-3.379	-4.207	-4.000e-06	0.00598	1.399	3.307
kag_000_19575	Br ₃ CaGd ₃ Tl	8	-3.029	-3.611	1.000e-05	0.00801	1.552	2.367
kag_000_19577	Ga ₂ MgNi ₃ Sn	7	-4.048	-4.131	-1.000e-06	0.00712	0.311	0.331
kag_000_19593	CoGaMgMn ₃ Zr	7	-6.38	-6.594	-2.500e-05	0.0059	0.195	0.466
kag_000_19621	Gd ₃ Se ₇ TiTl	12	-5.15	-5.327	1.000e-06	0.00409	0.586	0.395
kag_000_19626	Na ₅ Yb ₃	8	-1.28	-1.286	0.000e+00	0.00267	0.129	0.181
kag_000_19628	Cs ₃ Yb ₃	6	-0.78	-0.941	-2.500e-06	0.00141	1.415	1.192
kag_000_19696	Mg ₂ NdNi ₃	6	-4.137	-4.228	-8.000e-06	0.00752	0.218	0.203
kag_000_19712	Br ₄ ClCoGd ₃ Sn ₂ Ti	12	-3.631	-4.511	-1.000e-06	0.00569	1.614	3.466
kag_000_19713	Ge ₆ Mn ₅ Y	12	-6.607	-6.678	-5.100e-05	0.00366	0.183	0.598
kag_000_19724	AgCu ₂ Dy ₃ IS ₃ Sb	11	-3.995	-4.676	-6.100e-05	0.00689	2.146	3.558
kag_000_19752	Co ₆ Cu ₂	8	-5.82	-5.908	4.000e-06	0.00408	0.326	0.2
kag_000_19769	Na ₅ Yb ₃	8	-1.271	-1.283	-2.000e-06	0.00152	0.352	1.185
kag_000_19818	Co ₃ FeSm ₂	6	-6.403	-6.432	5.000e-06	0.00906	0.146	0.088
kag_000_19829	AlRu ₄ SnTh	7	-7.033	-7.555	-1.000e-06	0.00596	0.709	0.82
kag_000_19833	Co ₂ Mn ₄ NiSi	8	-7.465	-7.681	-5.000e-06	0.00776	0.41	0.266
kag_000_19842	Ni ₆ Pd ₂ Pr ₄	12	-5.436	-5.542	-1.690e-04	0.00838	0.454	0.477
kag_000_19844	CaGd ₃ LaNaSr ₂	8	-2.855	-2.929	0.000e+00	0.00326	0.251	0.42
kag_000_19855	Al ₃ Fe ₃ Tm ₃ U	10	-5.903	-6.21	-1.200e-05	0.00696	0.522	0.535
kag_000_19860	Ge ₄ LaNi ₄	9	-5.133	-5.203	1.000e-06	0.00963	0.583	1.056
kag_000_19872	HfPdRu ₃ Zr ₂	7	-8.771	-8.884	-4.000e-06	0.00929	0.379	0.434
kag_000_19896	KNaSbSnTb ₃	7	-3.21	-3.674	-4.000e-06	0.00343	1.593	2.918
kag_000_19958	Rh ₂ Sn ₇ Yb ₃	12	-3.962	-4.254	-2.000e-06	0.00664	1.025	2.096
kag_000_19979	Mn ₆ Si ₂ Zr ₄	12	-8.608	-8.688	0.000e+00	0.00249	0.223	0.165
kag_000_20032	Al ₂ Fe ₃ Ni ₃ Si ₂ Sn	11	-5.677	-5.919	0.000e+00	0.00818	0.372	1.704
kag_000_20077	BaBi ₃ EuGePbSr ₂ Tb ₃	12	-3.541	-3.925	0.000e+00	0.00453	1.548	1.216
kag_000_20101	La ₂ NaSrTl ₁ Yb ₃	8	-2.338	-2.394	-2.000e-06	0.00343	0.739	0.404
kag_000_20106	AlNi ₇	8	-5.315	-5.45	-7.000e-06	0.00538	0.343	0.859
kag_000_20118	CdGeNi ₃ PtSb	7	-4.478	-4.606	-6.700e-05	0.00793	0.753	2.22
kag_000_20124	CoGa ₄ Mn ₅ U ₂	12	-6.786	-7.178	0.000e+00	0.00973	0.847	1.465
kag_000_20126	AsFe ₃ Pt ₂ U	7	-7.222	-7.778	5.000e-06	0.00928	0.788	0.828
kag_000_20144	Dy ₃ Na ₂ Tl ₃	8	-2.793	-3.046	0.000e+00	0.00267	1.178	2.074
kag_000_20149	Gd ₃ InNa ₄	8	-2.617	-2.598	-2.000e-06	0.00549	0.505	0.425
kag_000_20160	Co ₈	8	-6.703	-6.839	1.000e-06	0.00496	0.383	0.919
kag_000_20163	Co ₃ Ge ₃ Tc	7	-6.214	-6.411	-2.300e-05	0.0076	0.715	2.46
kag_000_20180	BiLuNaPbSrTb ₃	8	-3.617	-3.783	-6.000e-06	0.00624	1.35	2.916
kag_000_20181	CaCl ₄ Gd ₃	8	-3.599	-4.146	-2.100e-05	0.00314	1.271	4.072
kag_000_20204	CaEu ₇ Gd ₃ Ge	12	-2.697	-2.795	-1.000e-06	0.00475	1.142	1.567
kag_000_20335	Ga ₂ HoIn ₂ Ni ₃	8	-4.05	-4.26	0.000e+00	0.00886	0.651	0.623
kag_000_20352	I ₂ Se ₅ SnTb ₃ Te	12	-4.297	-4.591	-2.000e-06	0.00209	1.159	1.544
kag_000_20391	Fe ₅ MnPt ₂	8	-7.26	-7.641	-5.000e-06	0.00525	0.772	1.793
kag_000_20395	MgSnTb ₃ Te ₃	8	-3.813	-4.588	-1.900e-05	0.00888	1.155	3.958
kag_000_20406	AuGa ₆ Yb ₅	12	-2.539	-2.793	-2.000e-06	0.00951	1.531	3.223
kag_000_20408	Ru ₄ Sn ₂ U	7	-7.713	-8.078	1.000e-06	0.00421	0.672	0.787
kag_000_20412	Cl ₅ CoGd ₃ Ir	10	-4.25	-5.188	-1.000e-06	0.00623	2.686	2.841
kag_000_20429	Ga ₄ Ni ₃ Sm	8	-4.277	-4.434	-8.000e-06	0.00704	0.504	0.66
kag_000_20439	CoFe ₃ Ni ₄	8	-6.313	-6.513	-3.500e-05	0.00526	0.15	0.291
kag_000_20464	CuGaNi ₆ PdUV ₂	12	-6.057	-6.207	-4.000e-06	0.00952	0.96	1.037
kag_000_20491	AuCl ₃ FGd ₃ GeI	10	-3.34	-4.627	-1.500e-05	0.00709	0.866	3.468
kag_000_20500	CaCd ₂ EuNd ₃ Sn	8	-2.999	-3.208	-1.000e-06	0.00361	1.698	3.185

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_20501	BaEuGdNd ₄ Sn	8	-3.772	-3.898	-1.000e-05	0.00352	0.954	0.491
kag_000_20535	CdGa ₂ LiNi ₃ Y	8	-4.114	-4.208	-4.000e-05	0.0068	0.322	0.398
kag_000_20559	Br ₈ PtYb ₃	12	-3.337	-3.504	-1.000e-06	0.00797	0.894	0.749
kag_000_20573	Co ₃ Dy ₂ Mn	6	-6.574	-6.63	-8.000e-06	0.00752	0.226	0.183
kag_000_20583	CrNiPt ₂ Ru ₄	8	-7.766	-7.934	-4.000e-06	0.00944	0.266	0.246
kag_000_20600	CoGe ₂ Mn ₄ Pt	8	-7.134	-7.238	1.000e-06	0.0078	0.537	1.0
kag_000_20623	Nb ₂ Ni ₅ Pt	8	-6.545	-6.965	5.000e-06	0.0094	0.744	1.703
kag_000_20624	AlNi ₈ Ta ₂ Zn	12	-6.144	-6.203	-2.000e-06	0.006	0.18	0.774
kag_000_20628	AuGaHf ₂ MgRu ₃ Sn ₃ Ti	12	-5.848	-6.45	0.000e+00	0.0068	1.142	1.79
kag_000_20659	Cs ₃ KYb ₃	7	-0.94	-0.965	8.300e-06	0.00328	0.527	0.567
kag_000_20669	AgGe ₂ Sb ₃ Tb ₄	10	-4.188	-4.833	-2.000e-06	0.00318	1.311	2.304
kag_000_20680	Co ₇ Pd	8	-6.329	-6.529	-6.000e-06	0.00933	0.709	0.552
kag_000_20684	Ga ₂ Pt ₃ Ru ₃	8	-6.539	-6.609	-3.000e-06	0.00466	0.15	0.089
kag_000_20721	NaTl ₄ Yb ₃	8	-1.86	-2.05	0.000e+00	0.00298	0.848	2.282
kag_000_20753	NaSn ₂ Tb ₃ Tl ₂	8	-3.602	-3.694	-1.400e-05	0.00478	0.35	0.316
kag_000_20754	AlFe ₇	8	-7.242	-7.634	0.000e+00	0.0057	0.23	1.056
kag_000_20763	CoFe ₇	8	-7.456	-7.924	-1.300e-05	0.00527	0.752	0.338
kag_000_20765	Cs ₃ Yb ₃	6	-0.598	-0.89	-5.450e-05	0.00404	2.272	2.922
kag_000_20772	DyGa ₃ Gd ₃ Sr	8	-3.528	-3.864	-2.000e-06	0.00863	0.733	1.868
kag_000_20786	Nd ₄ Sn ₂ Tl ₂	8	-3.996	-4.311	-1.000e-06	0.00938	0.602	1.407
kag_000_20815	BaMgSn ₃ Yb ₃	8	-2.528	-2.819	-1.000e-06	0.0041	1.253	3.294
kag_000_20838	NaTl ₄ Yb ₃	8	-1.824	-2.051	-1.000e-05	0.00464	0.841	1.418
kag_000_20845	Br ₄ ClDy ₃ Ru ₂	10	-4.221	-4.93	-3.000e-06	0.00523	1.479	2.051
kag_000_20849	InNa ₃ Yb ₄	8	-1.633	-1.535	5.000e-06	0.00351	1.808	2.635
kag_000_20857	Cs ₂ Nd ₃ Rb ₂	7	-1.995	-2.044	1.000e-06	0.00159	0.405	0.274
kag_000_20864	BaNaSnTb ₃ TlYb	8	-3.0	-3.238	0.000e+00	0.00362	2.151	2.032
kag_000_20881	K ₄ NaYb ₃	8	-0.997	-1.081	8.000e-07	0.0039	1.089	0.754
kag_000_20887	CoFe ₃ Mn ₃ Pt	8	-7.892	-7.991	-2.000e-06	0.00441	0.145	0.721
kag_000_20898	Dy ₃ EuGeNaPbTl	8	-3.079	-3.595	-1.000e-06	0.00655	1.904	1.279
kag_000_20914	As ₃ ClCrGa ₂ Gd ₄ Mn	12	-4.542	-5.442	-1.000e-06	0.00312	0.977	2.19
kag_000_20993	MgNbNi ₁₀	12	-5.579	-5.652	-5.000e-06	0.00708	0.288	0.267
kag_000_21016	CoMn ₄ O ₄ SrV	11	-4.891	-7.471	-1.600e-05	0.00851	0.711	1.558
kag_000_21041	Ni ₆ PtSb	8	-5.388	-5.433	-8.000e-06	0.00637	0.372	0.215
kag_000_21051	Pr ₄ Ru ₃	7	-6.341	-6.519	-5.700e-05	0.00944	0.278	0.301
kag_000_21060	Ba ₂ EuNaPbTb ₃	8	-2.888	-2.969	-1.000e-06	0.00385	0.484	1.496
kag_000_21061	Co ₈ Tm ₂	10	-6.002	-6.435	3.000e-06	0.00854	0.357	0.735
kag_000_21068	Ag ₂ Al ₂ Co ₄ La ₂	10	-4.491	-5.143	-6.000e-06	0.00905	1.519	1.706
kag_000_21072	In ₂ LuTb ₃ Tl ₂	8	-3.363	-3.733	-1.000e-06	0.00463	1.557	1.565
kag_000_21076	AsGeNi ₄ PtSi	8	-5.242	-5.563	-1.000e-06	0.00887	0.674	1.277
kag_000_21078	Al ₂ CoNi ₅	8	-5.428	-5.548	-1.000e-05	0.00696	0.528	0.915
kag_000_21093	Br ₃ NaSnYb ₃	8	-2.325	-3.178	-4.000e-06	0.00237	2.578	3.602
kag_000_21100	Br ₈ Gd ₃ Pb	12	-4.139	-4.051	-1.000e-06	0.0041	0.625	2.497
kag_000_21101	Tl ₅ Yb ₃	8	-1.972	-2.267	-2.000e-05	0.00414	1.367	0.956
kag_000_21116	Gd ₈	8	-4.561	-4.574	-1.600e-05	0.00207	0.148	0.159
kag_000_21133	Co ₅ Pt ₃	8	-6.412	-6.554	-1.100e-05	0.00676	0.341	0.207
kag_000_21151	AuEuGa ₃ Ni ₃	8	-3.715	-4.099	-4.000e-06	0.00984	1.173	0.874
kag_000_21185	Gd ₃ Na ₃ SnSr	8	-2.804	-2.894	-1.000e-06	0.00289	0.997	2.428
kag_000_21225	Co ₂ DyNi ₅	8	-5.528	-5.659	-1.000e-06	0.00503	0.84	2.371
kag_000_21228	CoMn ₆ Ni	8	-7.926	-8.233	-3.000e-06	0.00746	0.606	1.487
kag_000_21232	Tb ₃ Tl ₄	7	-2.94	-3.419	-2.000e-06	0.00341	1.032	0.96
kag_000_21247	MgTb ₃ Tl ₄	8	-2.937	-3.2	-2.000e-06	0.00508	0.717	1.376
kag_000_21266	Al ₅ Co ₃ Ti	9	-5.296	-5.585	-4.000e-06	0.00972	0.905	1.349

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_21270	Co ₆ Ge ₂ Sc ₄	12	-6.843	-6.87	-7.000e-06	0.00669	0.1	0.083
kag_000_21275	Na ₅ Yb ₃	8	-1.242	-1.286	-1.400e-05	0.00273	1.13	2.729
kag_000_21281	Nd ₆ Tl ₂	8	-4.147	-4.312	-9.000e-06	0.00263	0.457	0.406
kag_000_21285	BaCaDy ₄ Eu ₂ La ₄	12	-3.601	-3.64	-5.000e-06	0.00298	0.272	0.969
kag_000_21291	Ce ₄ EuTb ₃	8	-4.73	-4.747	0.000e+00	0.00579	0.144	0.114
kag_000_21318	Cl ₄ Fe ₂ LiNd ₃ Rb	11	-3.773	-4.528	0.000e+00	0.0075	2.161	2.539
kag_000_21319	Mn ₃ Pt ₅	8	-6.619	-7.146	-1.000e-05	0.0069	0.584	0.463
kag_000_21362	Mn ₃ Sn ₆	9	-4.869	-5.244	0.000e+00	0.00493	0.446	0.613
kag_000_21367	CaEuInNd ₅	8	-3.741	-3.792	-2.000e-06	0.00612	0.504	1.097
kag_000_21389	CrFe ₆ Pt	8	-7.867	-7.988	-5.000e-06	0.00765	0.273	0.258
kag_000_21406	Al ₄ Er ₄ Fe ₃	11	-5.245	-5.326	-9.600e-05	0.00686	0.201	0.235
kag_000_21440	Na ₅ Nd ₃	8	-2.281	-2.331	0.000e+00	0.00442	0.491	0.382
kag_000_21441	Al ₂ CeNi ₅	8	-5.06	-5.418	6.000e-06	0.00603	0.927	2.22
kag_000_21491	Dy ₃ Ga ₂ La ₃	8	-4.331	-4.506	-1.600e-05	0.0049	1.302	1.202
kag_000_21512	Gd ₄ NaSnSrTe	8	-3.565	-3.898	-5.000e-06	0.00206	1.74	2.308
kag_000_21535	BK ₂ Ru ₇ TeZr	12	-6.673	-6.991	-3.200e-05	0.00619	0.447	1.14
kag_000_21551	Br ₂ I ₂ RbSbTb ₃	9	-2.757	-3.858	-4.100e-05	0.00835	1.553	3.467
kag_000_21555	FePt ₄ Ru ₃	8	-7.337	-7.436	-2.700e-05	0.00642	0.261	0.205
kag_000_21595	Cl ₅ Ge ₂ SnYb ₃	11	-2.745	-3.812	-6.400e-05	0.0089	1.774	3.239
kag_000_21596	Gd ₃ Pb ₂ Th ₃	8	-5.537	-5.563	-1.000e-05	0.00392	0.192	1.013
kag_000_21597	Cs ₃ Dy ₃	6	-1.87	-2.035	-6.000e-06	0.00232	1.828	2.22
kag_000_21608	Co ₆ GaGe	8	-6.109	-6.199	1.000e-06	0.00959	0.423	0.334
kag_000_21628	EuGd ₅ In ₂	8	-3.901	-4.005	-4.000e-06	0.00381	0.333	0.158
kag_000_21647	CeGaSrTb ₃ Tl ₂	8	-3.511	-3.762	-2.000e-06	0.00595	1.549	2.258
kag_000_21659	AlNi ₅ Pt ₂	8	-5.428	-5.684	-6.000e-06	0.00618	0.688	0.513
kag_000_21673	CeMg ₂ Nd ₃ Tl ₂	8	-3.423	-3.583	2.000e-06	0.0083	0.517	0.25
kag_000_21703	CoMn ₃ Pt ₂ Si	7	-6.804	-7.4	-4.000e-06	0.00911	1.206	0.875
kag_000_21759	Na ₃ Sr ₂ Yb ₃	8	-1.37	-1.388	-1.000e-06	0.00322	1.401	1.833
kag_000_21761	Al ₂ Ni ₂ PdRu ₃	8	-6.591	-6.625	-1.000e-06	0.00675	0.155	0.759
kag_000_21776	Co ₄ GaMnY	7	-6.276	-6.625	1.000e-06	0.00699	0.352	0.476
kag_000_21781	Cs ₄ Dy ₃	7	-1.814	-1.849	-2.900e-05	0.00635	0.817	0.804
kag_000_21802	Ni ₈	8	-5.328	-5.41	-3.000e-06	0.0032	0.467	0.223
kag_000_21810	Fe ₄ Ni ₃ SiSn ₃	11	-5.486	-5.885	2.000e-06	0.00614	0.701	1.69
kag_000_21843	CrGeNi ₆	8	-5.909	-5.926	2.000e-06	0.005	0.134	0.113
kag_000_21845	Ga ₈ Mn ₃ U	12	-4.567	-5.066	-1.000e-06	0.00748	1.162	1.044
kag_000_21855	CoMn ₃ Pt ₂ SiTi	8	-7.48	-7.603	-1.200e-05	0.00968	0.291	1.4
kag_000_21859	As ₃ Co ₃ Na ₂ Sr	9	-3.898	-4.569	1.000e-06	0.00944	1.381	2.328
kag_000_21881	AcDy ₃ EuInNa ₂	8	-2.832	-2.983	0.000e+00	0.00599	1.505	1.16
kag_000_21914	Br ₈ SnTb ₃	12	-3.722	-4.041	-9.000e-06	0.00557	1.071	2.761
kag_000_21942	Dy ₃ Na ₄ Tl	8	-2.346	-2.501	-3.000e-06	0.0073	0.74	0.444
kag_000_21959	Br ₄ KMnYb ₃	9	-2.795	-3.144	5.000e-06	0.00921	1.885	1.671
kag_000_21960	Cl ₄ CsIrTb ₃	9	-3.84	-4.701	-3.700e-05	0.00606	1.481	4.897
kag_000_21964	Bi ₃ Yb ₅	8	-2.761	-2.968	-5.000e-06	0.00428	0.789	3.377
kag_000_21978	Cr ₄ Se ₅ Tb ₃	12	-5.633	-6.413	0.000e+00	0.00421	1.773	3.001
kag_000_21985	As ₃ Gd ₄ GeRh ₄	12	-5.941	-6.293	-9.000e-06	0.00723	0.935	2.109
kag_000_22046	Sb ₅ Tb ₃	8	-4.064	-4.985	-2.000e-06	0.00305	1.65	1.932
kag_000_22055	H ₄ Ni ₄	8	-3.46	-4.446	-3.800e-05	0.00572	1.305	2.025
kag_000_22079	Fe ₄ Sm ₂	6	-6.803	-6.835	-2.000e-06	0.00942	0.137	0.992
kag_000_22092	EuIn ₃ Ni ₄	8	-4.013	-4.136	-1.000e-06	0.0085	0.359	0.402
kag_000_22135	La ₂ Tb ₃ Tl ₃	8	-3.663	-4.034	1.000e-06	0.00469	0.811	0.61
kag_000_22138	PbPrSb ₂ Tb ₃	7	-4.521	-4.82	0.000e+00	0.00354	1.336	1.628
kag_000_22190	Na ₃ Yb ₅	8	-1.315	-1.326	-3.000e-06	0.00306	0.621	0.6

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_22245	BiP ₂ Ru ₆	10	-7.271	-8.187	1.000e-06	0.0051	0.596	0.79
kag_000_22266	Dy ₃ Na ₅	8	-2.195	-2.217	-2.000e-06	0.00329	0.911	1.376
kag_000_22305	CrFe ₃ Hf ₂	6	-9.076	-9.249	-1.000e-06	0.00461	0.486	0.327
kag_000_22326	K ₂ SbYb ₃	6	-1.66	-1.901	-3.000e-06	0.00285	1.505	1.246
kag_000_22344	Ce ₂ Fe ₃ Ru ₄	9	-8.04	-8.137	-1.100e-05	0.00779	0.236	0.8
kag_000_22353	Br ₅ OsTb ₃	9	-3.977	-4.64	-1.000e-06	0.00428	1.373	2.476
kag_000_22356	Cs ₄ Dy ₃	7	-1.8	-1.856	0.000e+00	0.00248	0.444	0.269
kag_000_22358	Co ₄ Ni ₃ U	8	-6.779	-6.99	-1.300e-05	0.00534	0.382	0.161
kag_000_22398	Br ₄ Gd ₃ K	8	-2.66	-3.673	0.000e+00	0.00359	2.367	3.334
kag_000_22418	Gd ₃ Na ₃ PbSr	8	-2.686	-2.784	-2.000e-06	0.00474	1.094	2.091
kag_000_22428	BaEu ₂ Na ₂ Tb ₃	8	-2.501	-2.521	-4.000e-06	0.00306	0.926	0.623
kag_000_22464	EuSn ₂ Sr ₂ Yb ₃	8	-2.216	-2.581	-1.000e-05	0.00708	1.045	1.313
kag_000_22478	InTb ₅ Tl ₂	8	-4.146	-3.998	-1.000e-06	0.00224	0.907	1.319
kag_000_22485	Br ₂ CrRh ₂ SeSnTe ₂ Yb ₃	12	-3.776	-4.599	-1.100e-05	0.0067	0.807	2.916
kag_000_22492	GaNi ₃ Pt ₄	8	-5.234	-5.649	-1.300e-05	0.00726	0.434	0.954
kag_000_22496	Mn ₃ Rh ₄ SiSn ₄	12	-5.819	-6.403	-9.000e-06	0.00864	1.04	1.928
kag_000_22502	Al ₂ NiRu ₅	8	-7.318	-7.55	1.000e-06	0.00946	0.52	0.886
kag_000_22553	Fe ₄ Pt ₄	8	-6.71	-6.96	1.000e-06	0.00604	0.368	0.81
kag_000_22569	CaGdSnSrTl ₂ Yb ₃	8	-2.296	-2.644	-2.800e-05	0.00365	2.163	3.376
kag_000_22625	AlNi ₅ Pt ₂	8	-5.661	-5.718	-1.400e-05	0.00958	0.419	0.19
kag_000_22628	BaLaNd ₃ Tl ₃	8	-3.366	-3.661	-3.000e-06	0.00707	1.211	3.651
kag_000_22641	CoNi ₄ Sn ₂	7	-4.94	-5.187	-6.000e-06	0.0093	1.311	1.5
kag_000_22675	Ni ₈	8	-5.406	-5.41	-3.000e-05	0.00542	0.062	0.686
kag_000_22739	Ni ₄ Pt ₄	8	-5.437	-5.785	-1.000e-06	0.0073	0.415	0.292
kag_000_22741	Cl ₄ IrRbYb ₃	9	-3.012	-3.959	1.000e-06	0.00442	1.244	4.697
kag_000_22745	Ni ₃ RhSe ₃	7	-4.683	-4.953	-7.600e-05	0.00894	1.082	1.09
kag_000_22754	Na ₅ Tb ₃	8	-2.21	-2.233	-3.000e-06	0.00288	0.897	1.228
kag_000_22768	Cr ₂ GeMn ₃ OsRe	8	-8.945	-9.123	-5.000e-06	0.00644	0.485	0.447
kag_000_22775	Ir ₄ Lu ₄ Mn ₄	12	-7.676	-7.939	-2.000e-06	0.00425	0.383	0.317
kag_000_22785	Ir ₄ NbSe ₄ Tb ₃	12	-6.377	-6.77	0.000e+00	0.0066	0.551	0.96
kag_000_22840	Al ₂ AuGd ₅ Si ₃	11	-4.588	-4.963	-1.000e-06	0.00364	1.066	2.327
kag_000_22893	Dy ₂ FeNi ₉	12	-5.561	-5.666	4.000e-06	0.00979	0.232	0.317
kag_000_23001	Br ₃ NaSnYb ₃	8	-2.305	-3.181	-1.000e-06	0.00459	2.872	4.081
kag_000_23022	Gd ₂ Mn ₃ Si	6	-6.815	-7.039	1.000e-06	0.00428	0.55	0.414
kag_000_23046	AlCrNi ₆	8	-5.835	-5.846	1.000e-05	0.00911	0.124	0.122
kag_000_23074	Co ₄ Mn ₄	8	-7.615	-7.939	0.000e+00	0.0083	0.378	0.226
kag_000_23079	Eu ₃ InNaYb ₃	8	-1.671	-1.792	0.000e+00	0.00456	1.663	3.683
kag_000_23087	Co ₃ CsSTe	6	-4.506	-5.051	-1.000e-06	0.00555	1.318	1.933
kag_000_23111	As ₂ Sr ₃ Tb ₃	8	-3.556	-3.965	-1.000e-05	0.00451	1.101	2.981
kag_000_23118	BrGeMgNd ₃ Pr ₂ Sn ₃ Yb	12	-3.931	-4.288	-3.000e-06	0.00602	1.621	3.202
kag_000_23131	EuGd ₃ In ₂ MgSr	8	-3.055	-3.205	-1.100e-05	0.00851	0.906	1.586
kag_000_23133	MgNi ₉ Ti ₂	12	-5.663	-5.889	-1.200e-05	0.00775	0.316	2.389
kag_000_23179	Na ₅ Nd ₃	8	-2.317	-2.328	-7.000e-06	0.00338	0.262	1.932
kag_000_23186	Al ₂ Ru ₄ Tm	7	-6.778	-7.288	-2.000e-06	0.00816	0.353	1.961
kag_000_23204	Al ₂ Fe ₇ Ti ₂ Zr	12	-7.196	-7.451	0.000e+00	0.00813	0.962	0.902
kag_000_23212	Fe ₃ NiPt ₄	8	-6.571	-6.689	-1.500e-05	0.00513	0.276	0.266
kag_000_23217	Tl ₄ Yb ₄	8	-1.935	-2.157	-2.000e-06	0.00218	0.811	0.528
kag_000_23247	Co ₂ Ni ₆	8	-5.641	-5.733	1.000e-06	0.00572	0.585	1.64
kag_000_23254	Fe ₄ HfNbPt	7	-8.256	-8.546	-8.000e-06	0.00451	0.351	0.259
kag_000_23259	Er ₂ Fe ₅ Ga ₃	10	-5.581	-5.953	-1.000e-06	0.00583	0.854	1.195
kag_000_23302	EuFe ₄ SnZn	7	-5.107	-5.419	-3.000e-06	0.00349	0.537	0.561
kag_000_23344	Dy ₃ Na ₅	8	-2.165	-2.216	1.000e-06	0.00214	0.377	0.254

Table S6. The profile of generated materials with Kagome lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
kag_000_23355	Co ₂ GeNi ₅	8	-5.439	-5.773	-4.000e-06	0.00607	0.814	1.079
kag_000_23367	Ni ₇ Tb	8	-5.28	-5.359	-1.600e-05	0.00833	0.43	0.422
kag_000_23378	Mn ₄ Si ₂ Tb	7	-7.066	-7.387	-2.000e-06	0.00502	0.465	1.16
kag_000_23387	Co ₇ Ti	8	-7.086	-7.144	-6.000e-06	0.00486	0.247	0.158
kag_000_23396	AsCdTb ₃ Tl ₂	7	-2.936	-3.801	3.000e-06	0.00546	1.314	1.096
kag_000_23397	BaK ₄ Ru ₃ Sn ₃	11	-3.791	-3.978	0.000e+00	0.00936	0.469	0.563
kag_000_23426	Al ₂ Fe ₃ Hf ₂ Ru ₃ TbU	12	-8.179	-8.252	2.000e-06	0.00837	0.307	0.442
kag_000_23431	Co ₆ GaGe	8	-6.032	-6.19	-6.000e-06	0.00713	0.519	0.929
kag_000_23447	Na ₅ Yb ₃	8	-1.282	-1.287	-1.000e-05	0.00233	0.155	0.106
kag_000_23491	Gd ₃ GeTl ₄	8	-3.505	-3.703	-6.000e-06	0.00395	0.62	1.777
kag_000_23499	AlCo ₅ MnSi	8	-6.702	-6.798	6.000e-06	0.00686	0.266	0.858
kag_000_23511	AlCa ₂ Ni ₃	6	-4.167	-4.3	-1.400e-05	0.00969	0.334	1.999
kag_000_23517	EuSn ₈ Yb ₃	12	-3.247	-3.512	-3.800e-05	0.00764	0.605	0.568
kag_000_23520	AlCoCuNi ₄ Rh	8	-5.564	-5.59	-3.200e-05	0.00308	0.199	1.365
kag_000_23566	K ₃ Na ₂ Tb ₃	8	-1.939	-1.959	-1.100e-05	0.00283	1.148	1.564
kag_000_23578	EuNa ₄ Nd ₃	8	-2.351	-2.443	-1.000e-06	0.00853	0.848	1.543
kag_000_23604	Al ₃ BeFeNi ₇	12	-5.372	-5.429	-1.400e-05	0.00775	0.219	0.288
kag_000_23640	Gd ₃ S ₅ V ₄	12	-6.037	-6.631	-4.000e-05	0.00702	0.68	0.538
kag_000_23642	AcKSb ₂ SrTb ₃	8	-3.447	-3.893	2.000e-06	0.00384	0.905	0.765
kag_000_23678	CaEu ₂ InNaNd ₃	8	-2.858	-2.958	1.000e-06	0.00444	0.699	1.491
kag_000_23690	Ga ₄ Nd ₄	8	-3.862	-4.352	0.000e+00	0.00817	0.788	1.861
kag_000_23705	Gd ₃ InLuTl ₃	8	-3.338	-3.686	-1.000e-06	0.00639	0.88	0.513
kag_000_23707	Gd ₆ Sr ₂	8	-3.65	-3.661	0.000e+00	0.0031	0.185	1.929
kag_000_23733	CrGe ₂ Mn ₃ PtSi	8	-6.799	-7.045	0.000e+00	0.00583	0.751	2.403
kag_000_23742	GaMn ₄ NiSn ₅	11	-4.989	-5.553	-4.300e-05	0.00933	0.794	0.963
kag_000_23745	Fe ₃ Ga ₂ GeHo	7	-5.435	-5.69	0.000e+00	0.00519	0.184	0.319
kag_000_23765	Fe ₅ Rh ₃	8	-7.401	-7.681	1.000e-06	0.00335	0.709	1.689
kag_000_23797	Fe ₄ NiPt ₃	8	-6.861	-6.946	-4.000e-06	0.0058	0.178	0.75
kag_000_23838	GeNd ₂ Ru ₃	6	-7.103	-7.269	-1.000e-06	0.00773	0.275	0.203
kag_000_23865	NaTl ₃ Yb ₄	8	-1.561	-1.909	-3.000e-06	0.00361	1.145	1.831
kag_000_23866	Ni ₃ SbScSe ₂	7	-4.745	-5.224	1.000e-06	0.00637	1.174	1.534
kag_000_23885	Co ₁₂	12	-6.749	-6.841	1.300e-05	0.00997	0.22	0.142
kag_000_23889	BrGd ₃ IrTe ₃ Tl	9	-4.327	-4.84	-1.100e-05	0.00785	2.217	2.755

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation

Index	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_00009	CoPt	2	-6.128	-6.49	-2.900e-05	0.00647	0.414	0.552
sqr_000_00010	CDy	2	-6.116	-6.838	-1.700e-05	0.004	0.867	0.631
sqr_000_00017	NiRh	2	-5.79	-6.322	-1.000e-05	0.00546	0.447	0.288
sqr_000_00019	CdGd	2	-2.984	-2.992	-8.000e-07	0.00063	0.06	0.049
sqr_000_00020	Ag ₂ PdYb	4	-3.391	-3.5	-2.000e-06	0.00238	0.301	0.206
sqr_000_00025	BeRu	2	-6.517	-6.679	-2.600e-05	0.0022	0.181	0.11
sqr_000_00031	DyZn	2	-3.161	-3.173	-8.600e-06	0.00533	0.064	0.04
sqr_000_00032	GdPt ₂	3	-6.064	-6.583	-4.000e-06	0.00496	0.427	0.371
sqr_000_00034	SYb	2	-4.34	-4.728	-1.000e-06	0.0025	0.424	0.328
sqr_000_00037	MnRu	2	-8.964	-8.985	-1.000e-06	0.0035	0.055	0.035
sqr_000_00041	MgNd	2	-3.192	-3.215	-1.850e-05	0.00022	0.271	0.226
sqr_000_00042	MgRu	2	-4.948	-5.112	0.000e+00	0.00161	0.261	0.163
sqr_000_00044	SbYb	2	-3.59	-3.593	-1.000e-06	0.00146	0.054	0.045
sqr_000_00045	TbTl	2	-3.728	-3.755	1.000e-07	0.00138	0.092	0.06
sqr_000_00049	GdSb	2	-5.172	-5.508	-1.000e-06	0.00018	1.437	0.954
sqr_000_00051	GdZn	2	-2.971	-3.192	-9.400e-06	0.0024	0.307	0.146
sqr_000_00052	GdMgSn ₂	4	-1.711	-3.854	0.000e+00	0.00882	0.65	0.485
sqr_000_00057	FeGdPtRh	4	-6.325	-6.781	0.000e+00	0.00896	0.286	0.275
sqr_000_00059	AgDy	2	-3.847	-3.973	-2.460e-05	0.00212	0.216	0.125
sqr_000_00069	SrYb	2	-1.428	-1.524	1.100e-06	0.00219	0.322	0.327
sqr_000_00076	MgYb	2	-1.512	-1.526	2.800e-05	0.00017	0.152	0.092
sqr_000_00078	MnPd	2	-6.717	-6.817	-1.400e-05	0.00429	0.201	0.169
sqr_000_00080	AgNd	2	-3.954	-3.996	-2.020e-05	0.00115	0.128	0.078
sqr_000_00083	RhRu	2	-7.761	-8.154	-4.000e-06	0.00999	0.373	0.228
sqr_000_00084	GaPYb	3	-3.773	-3.924	0.000e+00	0.00599	0.287	0.209
sqr_000_00087	SbYb	2	-3.589	-3.593	3.000e-07	0.00083	0.056	0.061
sqr_000_00097	HgYb	2	-1.357	-1.482	1.200e-06	0.00277	0.283	0.203
sqr_000_00098	RhYbZn ₂	4	-3.007	-3.062	0.000e+00	0.00641	0.14	0.109
sqr_000_00117	RhTb	2	-6.621	-6.752	-5.000e-06	0.00085	0.177	0.092
sqr_000_00122	BiNd	2	-5.055	-5.079	-2.600e-05	0.00739	0.422	0.299
sqr_000_00129	DyRu	2	-7.092	-7.18	8.000e-06	0.00045	0.144	0.13
sqr_000_00136	IrTb	2	-7.242	-7.499	-1.100e-05	0.00164	0.22	0.11
sqr_000_00138	DyRh	2	-6.716	-6.767	-1.000e-05	0.00344	0.105	0.075
sqr_000_00139	CuTb	2	-4.376	-4.394	-1.720e-05	0.00709	0.096	0.044
sqr_000_00144	NiSi	2	-5.71	-5.731	-5.000e-06	0.00732	0.139	0.121
sqr_000_00151	NiTb	2	-5.327	-5.399	-2.000e-05	0.00362	0.142	0.086
sqr_000_00153	GeNiTi	3	-6.007	-6.514	-3.000e-06	0.00437	0.678	0.578
sqr_000_00154	Ga ₂ RhYb	4	-3.924	-4.076	2.000e-06	0.00593	0.223	0.32
sqr_000_00157	GdS	2	-5.738	-6.042	-4.000e-06	0.00273	0.358	0.32
sqr_000_00158	AgGd	2	-3.963	-3.982	-2.300e-06	0.00441	0.081	0.067
sqr_000_00159	BeGd	2	-3.988	-4.044	-4.200e-06	0.00311	0.156	1.788
sqr_000_00161	DyS	2	-5.44	-6.325	0.000e+00	0.00133	0.789	0.415
sqr_000_00165	AgYb	2	-2.398	-2.527	-9.700e-06	0.00061	0.292	0.179
sqr_000_00166	DyLiPtRh	4	-5.526	-5.688	0.000e+00	0.0054	0.231	0.157
sqr_000_00169	GdRh ₂ Zn	4	-5.452	-5.655	0.000e+00	0.00504	0.307	0.266
sqr_000_00170	DyU	2	-6.807	-6.995	-7.000e-06	0.00106	0.409	0.318
sqr_000_00173	NiSi	2	-5.719	-5.729	-1.500e-05	0.00946	0.068	0.055
sqr_000_00174	DyGa ₂ Zr	4	-4.988	-5.174	-6.000e-06	0.00519	0.318	0.328
sqr_000_00175	AuYb	2	-3.152	-3.322	-4.000e-06	0.00179	0.301	0.307
sqr_000_00177	Nd ₂	2	-4.588	-4.703	4.000e-07	0.0004	0.51	0.453
sqr_000_00180	AgGd	2	-3.975	-3.984	-1.700e-06	0.0015	0.054	0.042
sqr_000_00185	CoZn	2	-3.91	-4.011	-7.600e-06	0.00576	0.33	0.246

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_00186	NdZn	2	-3.146	-3.223	-2.300e-06	0.00115	0.197	0.131
sqr_000_00187	DyPr	2	-4.477	-4.62	8.000e-07	0.00114	0.567	0.409
sqr_000_00188	DyTl	2	-3.537	-3.743	-1.300e-06	0.00212	0.294	0.132
sqr_000_00189	SeTb	2	-5.558	-5.558	0.000e+00	0.0001	0.008	0.013
sqr_000_00193	SeYb	2	-4.139	-4.563	-5.000e-07	0.00158	1.185	0.963
sqr_000_00196	GdMg	2	-3.096	-3.141	-2.010e-05	0.00341	0.15	0.12
sqr_000_00197	AgDy	2	-3.948	-3.971	1.200e-06	0.00181	0.078	0.045
sqr_000_00199	Ni ₂ PtTb	4	-5.667	-5.821	-6.000e-06	0.00725	0.176	0.148
sqr_000_00200	GdRu	2	-6.957	-7.144	-6.100e-05	0.00095	0.203	0.138
sqr_000_00202	GaTb	2	-4.276	-4.322	-2.000e-06	0.00566	0.13	0.09
sqr_000_00211	CdNd	2	-2.967	-3.059	1.400e-06	0.00247	0.198	0.133
sqr_000_00212	AlCu ₂ Nd	4	-3.594	-4.1	-5.000e-05	0.00678	0.887	0.729
sqr_000_00214	GdTe	2	-5.074	-5.086	-1.000e-06	0.00174	0.082	0.074
sqr_000_00216	SrYb	2	-1.109	-1.513	-1.300e-06	0.00171	0.586	0.428
sqr_000_00219	GdMg	2	-3.067	-3.14	1.000e-07	0.00319	0.176	0.108
sqr_000_00221	MnNi	2	-6.975	-7.145	2.000e-06	0.005	0.163	0.13
sqr_000_00222	AsNdPtRu	4	-6.484	-6.727	-1.000e-06	0.00462	0.293	0.395
sqr_000_00224	GdPd	2	-5.693	-5.751	-1.500e-05	0.0017	0.121	0.112
sqr_000_00225	GaTb ₃	4	-3.253	-4.389	-4.000e-06	0.00562	0.619	1.372
sqr_000_00226	CdNd	2	-3.026	-3.047	7.800e-06	0.00239	0.089	0.068
sqr_000_00230	NdZn	2	-2.986	-3.224	-3.900e-06	0.00134	0.335	0.216
sqr_000_00239	MgTb	2	-3.095	-3.122	-1.500e-06	0.00129	0.128	0.035
sqr_000_00241	FeRu	2	-8.398	-8.556	-7.000e-06	0.00271	0.131	0.098
sqr_000_00249	AlGd	2	-4.075	-4.565	-3.600e-06	0.00064	0.472	0.3
sqr_000_00251	CdTb	2	-2.945	-2.978	-3.800e-06	0.00294	0.105	0.063
sqr_000_00256	GdMg	2	-3.102	-3.14	1.000e-07	0.00077	0.128	0.05
sqr_000_00261	AlGaMgYb	4	-2.202	-2.615	-2.000e-06	0.00497	0.576	1.247
sqr_000_00273	BiYb	2	-3.301	-3.425	5.100e-06	0.00183	0.261	0.144
sqr_000_00274	CoGa	2	-4.988	-5.225	1.000e-06	0.00571	0.379	0.261
sqr_000_00275	MnTi	2	-8.357	-8.625	-5.200e-05	0.0039	0.171	0.076
sqr_000_00277	FeMn	2	-8.413	-8.53	-1.000e-05	0.00341	0.168	0.115
sqr_000_00278	GdPr	2	-4.053	-4.641	-3.200e-06	0.0012	0.499	0.896
sqr_000_00279	InYb	2	-2.508	-2.528	-1.000e-06	0.00171	0.101	0.058
sqr_000_00282	DyHg	2	-2.742	-2.849	-2.550e-05	0.00323	0.167	0.113
sqr_000_00283	NdPt	2	-6.328	-6.435	-3.000e-06	0.00516	0.159	0.1
sqr_000_00299	MgTb	2	-3.015	-3.119	-3.400e-06	0.00058	0.213	0.208
sqr_000_00304	DyTe	2	-4.859	-4.994	-1.900e-06	0.00021	0.216	0.125
sqr_000_00308	Nd ₂	2	-4.506	-4.7	1.000e-07	0.00223	0.591	0.586
sqr_000_00311	InYb	2	-2.51	-2.526	-8.100e-06	0.00223	0.107	0.077
sqr_000_00319	InRu	2	-5.338	-5.743	-1.500e-05	0.00367	0.269	0.201
sqr_000_00321	BiGd	2	-4.605	-4.97	-5.600e-06	0.005	0.434	0.302
sqr_000_00330	TlYb	2	-2.338	-2.342	-3.500e-06	0.00217	0.048	0.027
sqr_000_00331	SbTb	2	-5.0	-5.468	-1.000e-06	0.00079	1.453	1.191
sqr_000_00333	TlYb	2	-2.338	-2.341	-9.000e-07	0.00296	0.042	0.034
sqr_000_00335	AlFe	2	-6.076	-6.305	-3.000e-06	0.00258	0.427	0.293
sqr_000_00336	MnNi	2	-6.891	-7.131	-6.000e-06	0.00748	0.329	0.303
sqr_000_00340	GdZn	2	-3.186	-3.192	-1.000e-06	0.00396	0.053	0.054
sqr_000_00342	AuYb	2	-3.152	-3.321	-4.000e-06	0.00131	0.279	0.217
sqr_000_00343	PTb	2	-6.141	-6.269	0.000e+00	0.00241	0.153	0.132
sqr_000_00347	AuDy	2	-4.734	-4.759	-1.000e-07	0.00448	0.119	0.104
sqr_000_00349	NdSn	2	-4.708	-4.961	-7.500e-06	0.00362	0.509	0.485
sqr_000_00357	DySn	2	-4.737	-4.81	-6.900e-06	0.00561	0.381	0.269

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_00359	DyZn ₃	4	-2.074	-2.254	-5.000e-07	0.00262	0.8	0.666
sqr_000_00360	GdIn	2	-3.979	-3.923	-6.430e-05	0.00656	0.404	0.094
sqr_000_00363	HoTb	2	-4.349	-4.498	1.405e-04	0.00448	0.533	0.461
sqr_000_00371	NdTl	2	-3.677	-3.877	4.000e-07	0.00245	0.303	0.235
sqr_000_00375	RhTb	2	-6.688	-6.749	-6.000e-06	0.0014	0.186	0.081
sqr_000_00376	AuNi	2	-4.214	-4.248	2.600e-06	0.0023	0.11	0.134
sqr_000_00380	FeMg	2	-4.184	-4.317	-2.600e-06	0.00473	0.764	0.541
sqr_000_00389	AlRu	2	-7.073	-7.119	-5.000e-06	0.00073	0.077	0.079
sqr_000_00392	CoNd	2	-5.485	-5.779	-3.600e-05	0.00204	0.317	0.184
sqr_000_00393	NdSb	2	-4.88	-5.608	-1.000e-06	0.00346	1.463	0.964
sqr_000_00394	CdGd	2	-2.643	-3.006	-2.500e-06	0.00105	0.416	0.256
sqr_000_00396	DyZn	2	-3.167	-3.171	-4.100e-06	0.00319	0.049	0.038
sqr_000_00398	RuTb	2	-7.082	-7.156	-1.000e-06	0.00172	0.109	0.067
sqr_000_00402	FeRu	2	-8.358	-8.554	-1.200e-05	0.00403	0.154	0.14
sqr_000_00404	DyZr	2	-6.117	-6.354	-3.000e-06	0.00179	0.423	0.681
sqr_000_00415	RuTi	2	-8.679	-9.254	0.0000e+00	0.00137	0.525	0.437
sqr_000_00424	NiTi	2	-6.713	-6.989	2.000e-06	0.00601	0.327	0.231
sqr_000_00427	Gd ₂	2	-4.278	-4.554	-2.000e-07	0.00138	0.429	0.729
sqr_000_00429	DyHg	2	-2.751	-2.849	-7.200e-06	0.00358	0.161	0.128
sqr_000_00435	HgYb	2	-1.2	-1.5	-1.500e-06	0.00192	0.476	0.349
sqr_000_00436	PdRu	2	-6.678	-6.944	-8.000e-06	0.00264	0.524	0.587
sqr_000_00442	NiTi	2	-6.682	-6.976	5.000e-06	0.00231	0.371	0.187
sqr_000_00449	RuSi	2	-7.767	-7.945	-1.000e-06	0.00315	0.19	0.144
sqr_000_00453	CoNdY	3	-5.594	-6.02	-8.000e-06	0.00355	0.731	0.886
sqr_000_00455	CdNd	2	-2.877	-3.06	1.500e-06	0.00503	0.293	0.148
sqr_000_00456	InYb	2	-2.518	-2.526	-1.280e-05	0.00169	0.063	0.041
sqr_000_00460	NdSb	2	-5.097	-5.611	0.0000e+00	0.00125	1.288	1.171
sqr_000_00470	GdP	2	-6.076	-6.598	-1.000e-06	0.00201	1.268	0.943
sqr_000_00471	ScTb	2	-5.302	-5.35	0.0000e+00	0.00322	0.417	0.317
sqr_000_00473	CoRu	2	-7.764	-7.958	-2.800e-05	0.00351	0.317	0.173
sqr_000_00476	CeGdNa	3	-3.351	-3.718	-1.900e-05	0.00602	0.862	0.715
sqr_000_00479	PdRu	2	-6.621	-6.95	0.0000e+00	0.00231	0.574	0.505
sqr_000_00481	TeYb	2	-3.383	-3.97	-1.800e-06	0.00319	1.457	0.779
sqr_000_00482	GdZn	2	-3.189	-3.192	-2.800e-06	0.004	0.035	0.038
sqr_000_00490	AlMgYb	3	-2.195	-2.304	1.000e-07	0.00096	0.61	0.632
sqr_000_00497	CdYb	2	-1.496	-1.517	-1.000e-07	0.00279	0.117	0.08
sqr_000_00498	NiRh	2	-6.312	-6.318	-1.100e-05	0.00301	0.027	0.019
sqr_000_00500	MgTb	2	-3.093	-3.12	-1.550e-05	0.00047	0.287	0.179
sqr_000_00503	DyRh	2	-6.71	-6.767	-1.260e-04	0.0079	0.114	0.047
sqr_000_00506	TbTl ₃	4	-2.458	-3.031	1.000e-06	0.00445	0.428	0.246
sqr_000_00513	Cd ₂ GdMg	4	-1.48	-2.099	-5.000e-07	0.0032	0.89	0.459
sqr_000_00515	NiTi	2	-6.784	-6.99	-8.000e-06	0.00164	0.353	0.169
sqr_000_00518	HMn	2	-5.32	-6.198	0.0000e+00	0.00128	0.748	1.257
sqr_000_00520	MnRh	2	-7.662	-8.084	-1.000e-06	0.00381	0.481	0.318
sqr_000_00521	Ni ₂	2	-5.393	-5.414	-2.700e-05	0.0074	0.116	0.137
sqr_000_00522	AgTb	2	-3.953	-3.978	-1.000e-07	0.00123	0.085	0.069
sqr_000_00525	DyHg	2	-2.755	-2.849	-1.270e-05	0.00324	0.155	0.1
sqr_000_00526	CdTb	2	-2.974	-2.979	-1.300e-06	0.00306	0.028	0.03
sqr_000_00529	Ag ₂ Nd	3	-3.622	-3.657	-5.000e-06	0.00623	0.244	0.202
sqr_000_00531	FeRh	2	-7.563	-7.61	-1.000e-06	0.00207	0.075	0.059
sqr_000_00533	DyTe	2	-4.881	-4.992	-9.000e-07	0.00226	0.203	0.119
sqr_000_00534	BeNi	2	-5.059	-5.082	0.0000e+00	0.00156	0.059	0.021

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_00537	NiPt	2	-5.737	-5.857	-5.200e-05	0.00883	0.402	0.309
sqr_000_00539	RuTi	2	-9.233	-9.284	-7.900e-05	0.00534	0.099	0.066
sqr_000_00541	NdRh	2	-6.547	-6.613	-1.000e-05	0.00778	0.127	0.083
sqr_000_00548	GdSiTb	3	-4.049	-5.309	-9.000e-06	0.00604	1.344	0.575
sqr_000_00551	DyTe	2	-4.78	-5.101	-2.000e-06	0.00291	0.28	0.095
sqr_000_00552	AuTb	2	-4.728	-4.767	-2.800e-06	0.00203	0.106	0.083
sqr_000_00557	NdSb	2	-5.211	-5.611	0.000e+00	0.0011	1.306	0.899
sqr_000_00558	DySn	2	-4.319	-4.824	-1.020e-05	0.00158	0.663	1.103
sqr_000_00560	CuDy	2	-4.232	-4.398	-1.900e-06	0.002	0.242	0.113
sqr_000_00570	LiNd	2	-3.133	-3.165	-3.600e-06	0.00054	0.148	0.264
sqr_000_00577	CdNd	2	-3.019	-3.046	6.000e-06	0.00409	0.096	0.066
sqr_000_00581	FeIr	2	-8.377	-8.533	0.000e+00	0.00403	0.193	0.199
sqr_000_00586	AlFe	2	-5.961	-6.3	0.000e+00	0.00064	0.571	0.613
sqr_000_00587	GdTl	2	-3.583	-3.797	4.000e-07	0.00177	0.301	0.124
sqr_000_00589	AsTbZn	3	-4.142	-4.186	-2.000e-06	0.00753	0.148	0.154
sqr_000_00596	FeTi	2	-8.455	-8.459	-3.000e-06	0.00233	0.035	0.032
sqr_000_00597	RuSc	2	-8.15	-8.256	-2.100e-05	0.0022	0.136	0.086
sqr_000_00598	TbYb	2	-2.817	-2.851	-1.100e-06	0.0003	0.168	0.123
sqr_000_00599	HgTb	2	-2.704	-2.874	1.100e-06	0.00258	0.255	0.148
sqr_000_00601	MnSn	2	-4.963	-5.906	-4.000e-06	0.00229	1.013	0.755
sqr_000_00602	AuDy	2	-4.683	-4.761	-2.200e-06	0.00425	0.144	0.101
sqr_000_00606	YbZn	2	-1.528	-1.625	2.000e-07	0.001	0.254	0.213
sqr_000_00608	GdMg	2	-3.124	-3.141	2.200e-06	0.00285	0.215	0.221
sqr_000_00613	TIYb	2	-2.337	-2.342	-1.000e-07	0.00301	0.054	0.036
sqr_000_00616	NbNi	2	-7.735	-7.989	-1.900e-05	0.00737	0.204	0.162
sqr_000_00618	DyPd	2	-5.715	-5.76	-2.000e-06	0.0013	0.202	0.206
sqr_000_00619	CoTi	2	-7.468	-7.79	-4.700e-05	0.00622	0.422	0.296
sqr_000_00621	SeYb	2	-3.594	-4.262	-3.000e-07	0.00316	0.624	0.34
sqr_000_00622	GdSi ₂	3	-5.109	-5.691	-2.000e-06	0.00402	0.35	0.242
sqr_000_00626	CoTb	2	-5.727	-5.907	-1.800e-05	0.00188	0.225	0.106
sqr_000_00632	NiZn	2	-3.395	-3.539	-4.330e-05	0.00155	0.172	0.069
sqr_000_00633	TIYb	2	-2.298	-2.347	2.200e-06	0.00074	0.177	1.98
sqr_000_00635	AgDy	2	-3.925	-3.971	3.000e-07	0.00319	0.159	0.114
sqr_000_00639	EuYb	2	-1.474	-1.655	1.000e-07	0.00067	0.396	0.256
sqr_000_00643	HgNi	2	-2.215	-2.592	-7.000e-06	0.00545	0.247	0.137
sqr_000_00645	CdGd	2	-2.975	-2.999	-1.000e-07	0.00338	0.09	0.062
sqr_000_00648	AgYb	2	-2.442	-2.525	1.300e-06	0.00443	0.232	0.204
sqr_000_00653	NdZr	2	-6.283	-6.374	-2.400e-05	0.00158	0.496	0.472
sqr_000_00654	NiZn	2	-3.519	-3.542	-7.000e-07	0.00391	0.224	0.159
sqr_000_00655	GaHgLiNd	4	-2.473	-2.742	-1.000e-06	0.00323	0.493	0.282
sqr_000_00658	AgNd	2	-3.96	-3.994	-1.340e-05	0.00313	0.105	0.08
sqr_000_00660	HgTb	2	-2.805	-2.869	-1.200e-05	0.00242	0.145	0.091
sqr_000_00661	RuZn	2	-4.942	-4.994	-1.200e-06	0.00048	0.199	0.143
sqr_000_00662	RuZr	2	-9.457	-9.519	-7.000e-06	0.00089	0.131	0.099
sqr_000_00663	SmYb	2	-2.848	-2.939	-3.000e-07	0.00207	0.226	0.124
sqr_000_00667	NdSn	2	-4.944	-4.958	-3.300e-06	0.00058	0.074	0.045
sqr_000_00668	Ni ₂	2	-5.149	-5.401	-1.800e-05	0.00102	0.205	0.289
sqr_000_00669	GdZn ₃	4	-2.187	-2.191	5.300e-06	0.00311	0.039	0.041
sqr_000_00670	BeCo	2	-5.558	-5.697	0.000e+00	0.00048	0.231	0.335
sqr_000_00677	NdYb	2	-2.875	-2.994	-5.000e-06	0.0008	0.262	0.162
sqr_000_00681	AlFe	2	-6.226	-6.304	6.000e-06	0.00134	0.146	0.128
sqr_000_00683	FePt	2	-6.812	-7.065	-1.200e-05	0.0068	0.27	0.288

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_00685	TbZn	2	-3.181	-3.182	-2.100e-06	0.00092	0.016	0.014
sqr_000_00686	RhRu	2	-7.717	-8.143	1.000e-06	0.00268	0.442	0.227
sqr_000_00687	CuTb	2	-4.339	-4.394	-6.000e-06	0.0031	0.211	0.171
sqr_000_00688	NiRu	2	-7.098	-7.184	-8.000e-06	0.00569	0.081	0.039
sqr_000_00693	DySc	2	-5.259	-5.299	-6.000e-06	0.00173	0.125	0.048
sqr_000_00696	RuTb	2	-7.032	-7.163	-1.200e-05	0.00757	0.177	0.127
sqr_000_00701	Mg ₂ Yb	3	-1.443	-1.525	-4.000e-07	0.00145	0.515	2.196
sqr_000_00709	HgNd	2	-2.813	-2.918	-7.150e-05	0.00156	0.174	0.118
sqr_000_00714	CoMn	2	-7.908	-7.952	-1.900e-05	0.00517	0.105	0.095
sqr_000_00716	MnTi	2	-8.098	-8.632	-9.900e-05	0.00146	0.436	0.421
sqr_000_00717	CoGa	2	-5.229	-5.235	0.000e+00	0.00513	0.033	0.029
sqr_000_00721	AsYb	2	-3.864	-4.022	9.000e-07	0.00196	0.304	0.314
sqr_000_00723	MgNd	2	-3.167	-3.215	-9.600e-06	0.00106	0.155	0.022
sqr_000_00725	GdSi	2	-4.907	-5.483	-2.000e-05	0.00327	0.788	2.384
sqr_000_00726	SYb	2	-4.267	-4.728	-4.000e-07	0.00146	0.459	0.305
sqr_000_00727	AuYb	2	-3.157	-3.322	4.600e-06	0.00221	0.277	0.165
sqr_000_00732	GdPt	2	-6.478	-6.51	-3.000e-06	0.00389	0.087	0.042
sqr_000_00738	FePt	2	-7.031	-7.064	0.000e+00	0.00289	0.073	0.102
sqr_000_00740	BeMn	2	-6.226	-6.321	-5.400e-05	0.00076	0.151	0.134
sqr_000_00745	PtRu	2	-7.505	-7.595	0.000e+00	0.00444	0.189	0.179
sqr_000_00746	FeRu	2	-8.221	-8.551	-5.930e-04	0.00668	0.234	0.238
sqr_000_00747	AgNd	2	-3.899	-3.998	-3.370e-05	0.0063	0.198	0.13
sqr_000_00750	HoNdPbSb	4	-4.481	-4.847	-7.000e-06	0.00914	0.59	0.475
sqr_000_00751	MgRu	2	-5.099	-5.114	-1.000e-06	0.00416	0.069	0.069
sqr_000_00753	Ru ₂	2	-8.494	-9.091	4.000e-06	0.00309	0.178	0.343
sqr_000_00754	AlYb	2	-2.738	-2.793	2.400e-06	0.00094	0.181	0.08
sqr_000_00756	GdMoNi ₂	4	-5.844	-6.529	6.000e-06	0.00644	0.801	0.687
sqr_000_00761	TIYb	2	-2.332	-2.343	0.000e+00	0.00184	0.081	0.049
sqr_000_00765	GaTb	2	-4.168	-4.329	-3.200e-06	0.00351	0.245	0.138
sqr_000_00768	GaPd ₂ Yb	4	-4.304	-4.446	-4.000e-06	0.00591	0.48	0.371
sqr_000_00771	SYb	2	-4.348	-4.728	3.000e-07	0.00219	0.404	0.252
sqr_000_00772	AgAuDy	3	-4.095	-4.129	-1.000e-06	0.00331	0.136	0.079
sqr_000_00778	AlGdRh ₂	4	-5.837	-6.472	1.000e-06	0.00443	0.335	0.35
sqr_000_00779	NdTe	2	-5.086	-5.246	-4.000e-06	0.00289	0.229	0.173
sqr_000_00781	HgTb	2	-2.829	-2.863	-1.500e-06	0.00096	0.1	0.038
sqr_000_00788	GdYb	2	-2.787	-2.872	-2.300e-06	0.00172	0.215	0.143
sqr_000_00790	NdTl	2	-3.836	-3.873	5.800e-06	0.0018	0.12	0.049
sqr_000_00791	CDy	2	-6.305	-6.833	-1.000e-05	0.00481	0.656	1.936
sqr_000_00796	HoYb	2	-2.768	-2.791	2.235e-02	0.00806	0.144	0.085
sqr_000_00802	CoNi	2	-5.985	-6.074	-4.000e-06	0.00299	0.128	0.223
sqr_000_00804	AgYb	2	-2.452	-2.525	-4.000e-06	0.00189	0.215	0.18
sqr_000_00809	CoV	2	-8.024	-8.145	-1.400e-05	0.00723	0.121	0.114
sqr_000_00810	MnOs	2	-9.961	-10.02	0.000e+00	0.00317	0.071	0.063
sqr_000_00814	AlCuDyOs	4	-4.924	-5.939	-1.400e-05	0.00448	0.572	0.456
sqr_000_00817	CeYb	2	-3.283	-3.342	1.800e-06	0.0035	0.204	0.169
sqr_000_00818	Be ₃ Ni	4	-3.021	-4.467	0.000e+00	0.00306	0.624	0.357
sqr_000_00820	DySn	2	-4.806	-4.819	1.000e-07	0.00535	0.093	0.043
sqr_000_00827	GdTe	2	-4.994	-5.084	1.000e-06	0.00192	0.203	0.162
sqr_000_00828	BeFe	2	-5.973	-6.03	2.000e-06	0.00297	0.099	0.089
sqr_000_00829	GdIn	2	-3.976	-4.078	-5.500e-06	0.00105	0.198	0.136
sqr_000_00830	BiGd	2	-4.81	-4.951	-6.000e-07	0.00049	0.403	0.238
sqr_000_00832	YYb	2	-3.713	-3.787	1.580e-05	0.00359	0.203	0.137

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_00840	AuGaPdYb	4	-3.798	-3.896	-7.000e-06	0.00813	0.185	0.125
sqr_000_00842	NdSi	2	-5.404	-5.5	0.000e+00	0.0009	0.426	0.409
sqr_000_00845	NiZn	2	-3.448	-3.538	-1.740e-05	0.00128	0.158	1.556
sqr_000_00847	TbU	2	-6.817	-7.294	7.000e-06	0.00242	0.98	0.677
sqr_000_00848	PbYb	2	-2.779	-3.096	0.000e+00	0.00431	0.539	0.489
sqr_000_00852	CdDy	2	-2.946	-2.965	-4.300e-06	0.00334	0.08	0.059
sqr_000_00855	CoNiSi ₂	4	-6.116	-6.281	-9.000e-06	0.00555	0.452	0.448
sqr_000_00857	TlYb	2	-2.334	-2.342	-2.000e-07	0.00082	0.078	0.026
sqr_000_00860	STb	2	-5.905	-6.008	-1.000e-06	0.00262	0.165	0.1
sqr_000_00862	YbZn	2	-1.462	-1.625	-3.050e-05	0.00107	0.348	0.163
sqr_000_00865	SeYb	2	-3.807	-4.262	-6.900e-06	0.00106	0.491	0.332
sqr_000_00866	NdTl	2	-3.421	-3.877	7.000e-07	0.00238	0.511	0.487
sqr_000_00868	FeZn	2	-4.315	-4.344	1.720e-05	0.00296	0.09	0.07
sqr_000_00870	HGeLiTb	4	-2.766	-3.895	1.000e-06	0.00429	0.506	0.385
sqr_000_00872	AlNi	2	-4.717	-5.271	-3.000e-05	0.00338	0.414	0.275
sqr_000_00874	GdNd	2	-4.363	-4.648	3.800e-06	0.00149	0.54	0.503
sqr_000_00875	GdMg	2	-3.138	-3.14	-3.000e-06	0.00159	0.028	0.014
sqr_000_00876	CoTi	2	-7.501	-7.8	-4.400e-05	0.00222	0.51	0.545
sqr_000_00881	RuZr	2	-9.521	-9.523	-4.000e-06	0.00279	0.025	0.012
sqr_000_00882	CdDy	2	-2.913	-2.962	-9.600e-06	0.00387	0.12	0.092
sqr_000_00883	AlRu	2	-6.568	-7.153	-5.000e-06	0.00079	0.307	0.215
sqr_000_00884	RuSc	2	-8.106	-8.259	-1.400e-05	0.00216	0.175	0.155
sqr_000_00887	NdSb	2	-5.318	-5.598	-1.000e-06	0.00109	1.361	1.387
sqr_000_00889	Mn ₂	2	-8.871	-8.918	-3.000e-06	0.00127	0.157	0.157
sqr_000_00892	MnNi	2	-6.954	-7.126	-5.400e-05	0.00586	0.217	0.343
sqr_000_00894	GdTl	2	-5.852	-5.853	-1.000e-06	0.00061	0.013	0.017
sqr_000_00895	DySi	2	-5.401	-5.463	-1.000e-06	0.00232	0.33	0.206
sqr_000_00896	TbTe ₂	3	-4.564	-4.636	0.000e+00	0.00206	0.495	0.751
sqr_000_00899	Mg ₃ Yb	4	-1.198	-1.524	-2.000e-06	0.00154	1.2	0.729
sqr_000_00902	FeRu	2	-8.391	-8.557	4.000e-06	0.00096	0.15	0.078
sqr_000_00907	GdTl	2	-3.461	-3.79	-5.000e-07	0.0013	0.394	0.173
sqr_000_00910	NdSn	2	-4.658	-4.958	-5.100e-06	0.00127	0.682	0.668
sqr_000_00911	SbYb	2	-3.589	-3.593	-6.300e-06	0.00237	0.043	0.041
sqr_000_00912	DySbZn ₂	4	-3.059	-3.142	-2.000e-06	0.00361	0.195	0.216
sqr_000_00919	GdIn	2	-3.941	-4.078	1.000e-07	0.00075	0.256	0.071
sqr_000_00923	DyPd	2	-5.755	-5.762	-1.500e-05	0.00486	0.079	0.069
sqr_000_00928	ErYb	2	-2.735	-2.787	7.400e-06	0.00204	0.171	0.119
sqr_000_00931	NdS	2	-6.106	-6.154	0.000e+00	0.00138	0.117	0.093
sqr_000_00936	CaTb	2	-3.047	-3.066	-3.200e-06	0.00061	0.111	0.05
sqr_000_00937	NdTe	2	-4.772	-5.252	0.000e+00	0.00832	0.455	0.29
sqr_000_00938	GdYb	2	-2.818	-2.874	-1.900e-06	0.0008	0.175	0.097
sqr_000_00940	DyTe	2	-4.877	-4.998	-4.700e-06	0.00501	0.224	0.243
sqr_000_00944	GeMgTb	3	-2.515	-3.992	-3.000e-06	0.00595	0.38	0.866
sqr_000_00946	MgNd	2	-3.175	-3.215	1.100e-06	0.00629	0.143	0.169
sqr_000_00947	NdTe	2	-4.727	-5.252	0.000e+00	0.00039	0.509	0.395
sqr_000_00950	YbZn	2	-1.525	-1.625	2.200e-06	0.00359	0.258	0.172
sqr_000_00952	DyNd	2	-4.486	-4.612	1.000e-06	0.00149	0.582	0.333
sqr_000_00954	AlCo	2	-5.89	-5.991	-2.000e-06	0.00108	0.153	0.115
sqr_000_00958	GdNd	2	-4.17	-4.643	-6.700e-06	0.00299	0.468	0.396
sqr_000_00961	TlYb	2	-1.98	-2.363	-1.120e-05	0.00161	0.585	0.431
sqr_000_00965	PdYb	2	-3.966	-4.203	2.000e-07	0.00082	0.372	0.235
sqr_000_00966	MnRu	2	-8.695	-8.981	-3.000e-05	0.00363	0.43	0.338

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_00968	HgNd	2	-2.593	-2.942	-4.100e-06	0.00127	0.4	0.305
sqr_000_00970	AgNdTcZr	4	-6.237	-6.415	-2.000e-06	0.00486	0.941	0.659
sqr_000_00974	DyTb	2	-4.165	-4.493	-5.200e-06	0.00424	0.403	0.357
sqr_000_00980	MgRu	2	-5.049	-5.12	-3.000e-06	0.00088	0.126	0.072
sqr_000_00983	FeRh	2	-7.448	-7.613	-1.000e-06	0.00377	0.203	0.235
sqr_000_00984	AuCdGd	3	-3.351	-3.389	0.000e+00	0.00332	0.314	0.227
sqr_000_00985	GdMg	2	-3.048	-3.141	-6.600e-06	0.00039	0.22	0.182
sqr_000_01000	AuNd	2	-4.605	-4.756	-3.400e-06	0.00328	0.218	0.091
sqr_000_01005	NiTi	2	-6.686	-6.975	-1.000e-05	0.00367	0.456	0.39
sqr_000_01008	MgNd	2	-3.159	-3.217	-4.500e-06	0.00048	0.175	0.136
sqr_000_01009	NdTb	2	-4.068	-4.607	5.600e-06	0.00464	0.442	0.361
sqr_000_01011	DyMg	2	-3.026	-3.099	-1.520e-05	0.00148	0.17	0.098
sqr_000_01016	NiPd	2	-5.013	-5.264	1.000e-06	0.00241	0.173	0.108
sqr_000_01026	HfRu	2	-10.363	-10.372	0.000e+00	0.00121	0.038	0.03
sqr_000_01028	HfNi	2	-7.741	-8.124	2.000e-06	0.00399	0.328	0.164
sqr_000_01029	AlNd	2	-4.52	-4.578	-8.000e-07	0.00082	0.145	0.09
sqr_000_01034	GaMn	2	-5.735	-5.798	3.000e-06	0.00181	0.466	0.53
sqr_000_01037	AlFe	2	-6.19	-6.303	-1.000e-05	0.00477	0.237	0.335
sqr_000_01038	RuTb	2	-6.148	-7.109	-2.000e-06	0.00158	0.32	0.197
sqr_000_01039	FeIr	2	-8.036	-8.538	-7.000e-06	0.00488	0.455	0.255
sqr_000_01040	Br ₂ Ru	3	-3.054	-3.863	-6.000e-06	0.00798	0.733	0.901
sqr_000_01041	AuRu	2	-5.396	-5.662	-6.000e-06	0.00033	0.234	0.348
sqr_000_01043	NdZr	2	-6.268	-6.335	6.000e-06	0.00117	0.293	0.147
sqr_000_01045	SbYb	2	-3.584	-3.592	-1.000e-06	0.00239	0.07	0.061
sqr_000_01047	GdTe	2	-5.009	-5.084	-2.000e-06	0.00384	0.148	0.06
sqr_000_01048	HfNd	2	-6.872	-6.925	-2.000e-06	0.00397	0.123	0.08
sqr_000_01049	RuTi	2	-9.261	-9.276	-7.000e-06	0.00292	0.041	0.026
sqr_000_01051	RhSbTbTi	4	-5.653	-6.438	-1.000e-06	0.00398	0.525	1.176
sqr_000_01053	CoRe	2	-9.476	-9.674	-9.000e-06	0.00463	0.126	0.153
sqr_000_01054	AlFeGdRe	4	-6.389	-7.064	-1.400e-05	0.00769	0.608	0.658
sqr_000_01055	CdNd	2	-2.846	-3.061	1.900e-06	0.00147	0.324	0.25
sqr_000_01057	MgNd	2	-3.16	-3.217	-8.000e-06	0.00112	0.179	0.135
sqr_000_01058	MgNaRhYb	4	-2.553	-2.94	0.000e+00	0.0036	0.819	0.615
sqr_000_01061	Sn ₃ Tb	4	-1.795	-4.281	0.000e+00	0.00314	0.598	0.505
sqr_000_01062	GaRu	2	-6.05	-6.318	0.000e+00	0.00236	0.487	0.439
sqr_000_01063	NdZr	2	-6.278	-6.383	0.000e+00	0.00261	0.527	0.426
sqr_000_01065	AgDy	2	-3.948	-3.973	-7.000e-07	0.00073	0.101	0.075
sqr_000_01068	BeNi	2	-4.863	-5.083	-3.000e-06	0.00263	0.197	0.169
sqr_000_01070	BrGd	2	-3.929	-3.932	-8.000e-07	0.00783	0.051	0.05
sqr_000_01071	MgRu	2	-5.059	-5.12	-1.100e-05	0.00104	0.117	0.081
sqr_000_01073	ErNd	2	-4.152	-4.585	-1.200e-06	0.00044	0.507	0.974
sqr_000_01074	ErNd	2	-4.528	-4.584	2.000e-07	0.00217	0.252	0.192
sqr_000_01075	GdYb	2	-2.835	-2.875	-1.400e-06	0.00282	0.157	0.129
sqr_000_01078	NdS ₂ Sm	4	-6.336	-6.423	-1.000e-06	0.00327	0.385	0.361
sqr_000_01079	NaTb	2	-2.264	-2.495	-3.000e-07	0.00027	0.371	0.316
sqr_000_01081	MnNi	2	-6.816	-7.117	1.000e-06	0.00246	0.482	0.275
sqr_000_01085	IrRh ₂ Tb	4	-6.218	-7.274	-1.000e-05	0.00745	0.361	0.21
sqr_000_01089	FeIr	2	-8.279	-8.526	7.000e-06	0.00817	0.234	0.119
sqr_000_01091	RuTb	2	-7.129	-7.152	0.000e+00	0.00216	0.06	0.031
sqr_000_01093	YbZn	2	-1.533	-1.625	-5.000e-06	0.00285	0.256	0.085
sqr_000_01096	GaNdNiZr	4	-5.044	-5.732	3.000e-06	0.00554	0.615	0.716
sqr_000_01099	AgAlCaNd	4	-3.498	-3.562	-3.000e-06	0.00294	0.321	0.388

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_01101	SbTb	2	-4.685	-5.495	0.000e+00	0.00028	1.344	0.808
sqr_000_01102	DyIn	2	-3.924	-4.017	-7.000e-07	0.00325	0.165	0.095
sqr_000_01105	AlRu	2	-7.068	-7.135	-8.000e-06	0.00079	0.094	0.06
sqr_000_01109	PtRu	2	-7.084	-7.58	-8.000e-06	0.00165	0.531	0.368
sqr_000_01115	Ni ₂	2	-5.312	-5.415	-1.000e-06	0.00348	0.193	0.148
sqr_000_01118	NdSn ₃	4	-3.386	-4.504	-6.000e-06	0.00949	0.515	0.409
sqr_000_01119	YbZn	2	-1.529	-1.624	-1.000e-07	0.00172	0.25	0.211
sqr_000_01120	AgNd	2	-3.981	-3.993	1.900e-06	0.00128	0.08	0.047
sqr_000_01122	NiRu	2	-7.004	-7.188	-1.400e-05	0.00277	0.437	0.327
sqr_000_01129	DyZn	2	-2.98	-3.172	-1.250e-05	0.00369	0.28	0.215
sqr_000_01134	NdZn	2	-3.223	-3.224	2.000e-07	0.00178	0.017	0.017
sqr_000_01140	FeNi	2	-6.579	-6.643	-1.700e-05	0.00479	0.099	0.092
sqr_000_01149	GdIr ₃	4	-6.953	-7.977	-4.000e-06	0.00228	0.417	0.257
sqr_000_01153	Ga ₂ MgTb	4	-3.306	-3.434	1.000e-06	0.00821	0.234	0.161
sqr_000_01156	MgTb	2	-3.115	-3.122	-8.100e-06	0.00081	0.056	0.039
sqr_000_01159	DyTe	2	-4.828	-4.994	-4.000e-07	0.0036	0.245	0.096
sqr_000_01160	MgYb	2	-1.515	-1.529	-5.000e-07	0.00216	0.177	0.137
sqr_000_01165	AlGd	2	-4.214	-4.565	-3.000e-07	0.00031	0.432	0.295
sqr_000_01166	GaRu	2	-6.024	-6.345	-2.000e-06	0.00227	0.226	0.134
sqr_000_01168	GdSn	2	-4.606	-4.872	9.100e-06	0.0023	0.512	0.384
sqr_000_01174	GdRh	2	-6.503	-6.72	0.000e+00	0.00773	0.229	0.139
sqr_000_01175	RuYb	2	-5.122	-5.126	1.000e-06	0.00155	0.048	0.051
sqr_000_01176	MnRu	2	-8.521	-8.967	0.000e+00	0.00448	0.196	0.241
sqr_000_01179	MgRu	2	-4.9	-5.117	-4.000e-06	0.00039	0.224	0.133
sqr_000_01180	DyEr	2	-4.041	-4.445	-1.000e-06	0.00273	0.352	0.3
sqr_000_01181	RuTc	2	-9.265	-9.733	1.400e-05	0.00437	0.235	0.394
sqr_000_01184	BiDy	2	-4.8	-4.886	-1.360e-05	0.00104	0.324	0.156
sqr_000_01187	CrGdMnSb	4	-6.124	-6.422	-2.000e-06	0.00652	0.344	0.341
sqr_000_01188	MgTb	2	-2.993	-3.119	-3.800e-06	0.00205	0.229	0.065
sqr_000_01191	RuV	2	-8.972	-9.316	0.000e+00	0.00236	0.302	0.16
sqr_000_01193	PdRu	2	-6.704	-6.947	1.000e-06	0.00277	0.544	1.665
sqr_000_01197	MoRu	2	-9.797	-10.025	-4.000e-06	0.00286	0.132	0.127
sqr_000_01198	TbTl	2	-3.687	-3.753	3.000e-07	0.00143	0.26	0.205
sqr_000_01203	CdYb	2	-1.498	-1.518	0.000e+00	0.00269	0.102	0.081
sqr_000_01206	AuNd	2	-4.741	-4.748	1.000e-07	0.00272	0.063	0.047
sqr_000_01207	TbTl	2	-3.703	-3.764	-3.700e-06	0.00085	0.16	0.093
sqr_000_01210	AlDy	2	-4.454	-4.54	0.000e+00	0.002	0.174	0.101
sqr_000_01213	DyMg	2	-3.071	-3.103	-7.000e-07	0.00306	0.123	0.092
sqr_000_01216	CdNd	2	-2.996	-3.044	-3.700e-06	0.00449	0.121	0.071
sqr_000_01217	NdYb	2	-2.895	-2.994	-1.900e-06	0.00032	0.239	0.162
sqr_000_01218	DyY	2	-5.34	-5.459	3.000e-06	0.00035	0.602	0.444
sqr_000_01223	NdPd	2	-5.7	-5.703	-1.000e-06	0.00184	0.035	0.021
sqr_000_01226	DyY	2	-5.038	-5.449	0.000e+00	0.00216	0.4	0.763
sqr_000_01228	CoFe	2	-7.389	-7.458	0.000e+00	0.00253	0.142	0.188
sqr_000_01229	GaNd	2	-4.347	-4.371	-2.200e-06	0.00307	0.093	0.07
sqr_000_01232	DyTl	2	-3.719	-3.732	-1.700e-06	0.00298	0.067	0.051
sqr_000_01233	BiDy	2	-4.784	-4.882	-2.520e-05	0.00091	0.42	0.399
sqr_000_01235	DyLi	2	-3.028	-3.064	-4.000e-07	0.00149	0.149	0.077
sqr_000_01236	DyMg	2	-3.043	-3.099	-1.050e-05	0.00066	0.164	0.072
sqr_000_01239	FeZn	2	-4.269	-4.337	5.000e-06	0.00039	0.176	0.162
sqr_000_01241	PdTb	2	-5.646	-5.752	-7.000e-06	0.00161	0.165	0.105
sqr_000_01242	DyPt ₃	4	-6.243	-6.713	-8.000e-06	0.00436	0.263	0.22

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_01256	NiPd	2	-5.246	-5.275	-1.000e-06	0.00731	0.096	0.084
sqr_000_01257	Ni ₂	2	-5.341	-5.408	-2.000e-06	0.00237	0.121	0.169
sqr_000_01258	NiPd	2	-5.084	-5.271	-3.000e-06	0.00339	0.186	0.059
sqr_000_01261	HgNd	2	-2.785	-2.933	-2.060e-05	0.0011	0.245	0.206
sqr_000_01268	RhRu	2	-7.195	-8.226	-1.000e-06	0.00646	0.493	0.293
sqr_000_01269	CdDy	2	-2.853	-2.959	-3.210e-05	0.00464	0.174	0.105
sqr_000_01277	CoOsSi	3	-7.26	-8.019	-1.000e-06	0.0061	0.285	0.143
sqr_000_01278	Au ₃ Nd	4	-3.938	-4.087	-1.000e-06	0.0082	0.22	0.227
sqr_000_01295	P ₂ Tb	3	-5.66	-5.862	1.000e-06	0.00324	0.298	0.159
sqr_000_01296	MnNb	2	-9.173	-9.72	-1.000e-06	0.00171	0.496	0.395
sqr_000_01297	PbTb	2	-4.453	-4.515	-3.000e-07	0.00516	0.44	0.205
sqr_000_01303	CaYb	2	-1.479	-1.676	4.000e-06	0.00093	0.457	0.878
sqr_000_01304	InYb	2	-2.513	-2.527	-1.360e-05	0.00292	0.1	0.089
sqr_000_01306	CdGd	2	-2.839	-3.003	-1.500e-06	0.00395	0.257	0.15
sqr_000_01307	AgGd	2	-3.944	-3.983	2.000e-07	0.00198	0.121	0.089
sqr_000_01309	FeRh	2	-7.16	-7.621	-3.000e-06	0.00136	0.474	0.3
sqr_000_01310	GdLi	2	-3.092	-3.098	-4.700e-06	0.00453	0.053	0.098
sqr_000_01316	LiNdZn ₂	4	-1.962	-2.343	-1.040e-05	0.0071	0.821	0.612
sqr_000_01318	RuTi	2	-9.273	-9.279	0.000e+00	0.00048	0.039	0.026
sqr_000_01320	FeZn	2	-4.301	-4.319	-1.700e-06	0.00252	0.067	0.061
sqr_000_01325	CoV	2	-7.949	-8.158	-9.000e-06	0.00259	0.378	0.318
sqr_000_01334	AuNd	2	-4.746	-4.751	-8.060e-05	0.00531	0.033	0.028
sqr_000_01338	RuTi	2	-9.167	-9.27	0.000e+00	0.00172	0.154	0.121
sqr_000_01340	CoRu	2	-7.722	-7.944	-8.000e-06	0.00935	0.185	0.166
sqr_000_01343	RuV	2	-9.137	-9.322	-6.000e-06	0.00223	0.488	0.579
sqr_000_01351	Ga ₂ NbNd	4	-4.519	-5.267	1.000e-06	0.00421	0.446	0.271
sqr_000_01355	RuTi	2	-8.784	-9.253	-5.000e-06	0.00503	0.315	0.222
sqr_000_01356	InYb	2	-2.511	-2.526	1.640e-05	0.00249	0.109	0.109
sqr_000_01366	YYb	2	-3.721	-3.788	-1.300e-06	0.00094	0.19	0.135
sqr_000_01367	HfRu	2	-9.895	-10.355	-1.000e-06	0.00182	0.2	0.081
sqr_000_01369	CoMn	2	-7.603	-7.959	-2.000e-06	0.00337	0.26	0.268
sqr_000_01371	CoFe	2	-7.081	-7.458	1.000e-06	0.00318	0.484	0.328
sqr_000_01374	SmYb	2	-2.901	-2.939	-1.100e-06	0.00329	0.155	0.113
sqr_000_01375	MgNd	2	-3.14	-3.217	-2.800e-06	0.00136	0.204	0.098
sqr_000_01376	IrPtSnYb	4	-5.224	-5.645	0.000e+00	0.00344	0.407	0.416
sqr_000_01378	CuNi	2	-4.487	-4.554	-5.000e-06	0.00528	0.186	0.15
sqr_000_01379	RuV	2	-8.902	-9.314	-1.900e-05	0.00408	0.286	0.2
sqr_000_01381	DyGd	2	-4.313	-4.521	-6.000e-07	0.00025	0.5	0.545
sqr_000_01384	GdMg	2	-3.12	-3.141	1.800e-06	0.00076	0.102	0.068
sqr_000_01387	CoTi	2	-7.363	-7.786	3.000e-06	0.00386	0.624	0.355
sqr_000_01388	AuRu	2	-5.613	-5.633	0.000e+00	0.00302	0.059	0.054
sqr_000_01393	Nd ₂	2	-4.645	-4.703	1.200e-06	0.00284	0.206	0.227
sqr_000_01394	PdRu	2	-6.734	-6.949	4.000e-06	0.00379	0.417	0.495
sqr_000_01396	DyMg	2	-3.058	-3.099	-2.200e-06	0.00026	0.131	0.077
sqr_000_01400	DySc	2	-5.084	-5.317	-2.000e-06	0.0005	0.3	0.22
sqr_000_01408	PtTb	2	-6.505	-6.521	-7.000e-06	0.00385	0.056	0.028
sqr_000_01409	AuYb	2	-3.15	-3.322	3.000e-07	0.0037	0.282	0.168
sqr_000_01410	RuZr	2	-9.516	-9.524	-1.000e-06	0.00321	0.028	0.021
sqr_000_01412	PdTb	2	-5.75	-5.757	1.000e-06	0.00367	0.055	0.058
sqr_000_01413	GdSn	2	-4.779	-4.868	-1.880e-05	0.00157	0.454	0.252
sqr_000_01415	SeYb	2	-3.925	-4.262	-2.100e-06	0.00455	0.406	0.283
sqr_000_01421	Mg ₂ SnTb	4	-2.838	-3.272	-2.000e-06	0.00328	0.415	0.418

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_01424	Yb ₂	2	-1.299	-1.447	2.000e-07	0.00246	0.343	0.169
sqr_000_01425	AuNd	2	-4.694	-4.75	1.500e-06	0.00172	0.164	0.14
sqr_000_01432	DySr	2	-2.776	-2.8	-9.670e-05	0.0021	0.135	0.184
sqr_000_01434	AlRu	2	-6.846	-7.131	-1.000e-06	0.00089	0.33	0.517
sqr_000_01435	MnZn	2	-4.554	-4.797	-1.110e-05	0.00375	0.53	0.46
sqr_000_01440	HMn	2	-5.13	-5.73	1.000e-06	0.00038	0.403	0.208
sqr_000_01443	CoPt	2	-6.398	-6.488	0.000e+00	0.00495	0.103	0.102
sqr_000_01448	CoNi	2	-5.934	-6.062	1.000e-06	0.00275	0.395	0.23
sqr_000_01449	CoMn	2	-7.638	-7.948	-1.800e-05	0.00394	0.354	0.415
sqr_000_01450	CdGd	2	-2.964	-2.999	-2.900e-06	0.00341	0.118	0.051
sqr_000_01455	CoNi	2	-5.927	-6.06	-7.000e-06	0.00202	0.375	0.401
sqr_000_01456	InYb	2	-2.513	-2.528	-1.120e-05	0.00258	0.09	0.035
sqr_000_01458	NdPd	2	-5.408	-5.694	-1.000e-06	0.00334	0.308	0.232
sqr_000_01460	NdTl	2	-3.867	-3.868	7.900e-06	0.00129	0.032	0.031
sqr_000_01461	DySm	2	-4.205	-4.566	3.800e-06	0.00216	0.438	0.737
sqr_000_01462	Au ₂ TiYb	4	-4.022	-4.489	-1.000e-06	0.00936	0.767	0.688
sqr_000_01470	GdSr	2	-2.596	-2.843	-2.510e-05	0.00078	0.426	0.319
sqr_000_01472	Ag ₂ TbZr	4	-4.729	-4.763	-3.000e-06	0.00164	0.133	0.182
sqr_000_01476	SbYb	2	-3.59	-3.591	-3.300e-06	0.0028	0.045	0.032
sqr_000_01477	GdTe	2	-4.864	-5.088	-8.000e-06	0.00091	0.284	0.153
sqr_000_01479	AgNd	2	-3.8	-4.001	-3.300e-06	0.00107	0.295	0.173
sqr_000_01480	HgYb	2	-1.435	-1.476	1.600e-06	0.00303	0.15	0.146
sqr_000_01481	AsFe	2	-5.795	-6.308	0.000e+00	0.0038	0.649	0.53
sqr_000_01482	GdZr	2	-6.175	-6.366	1.000e-05	0.00194	0.463	0.662
sqr_000_01487	GdRh	2	-6.647	-6.729	-3.000e-06	0.00649	0.145	0.093
sqr_000_01490	PTb	2	-5.896	-6.593	-2.000e-06	0.00039	1.282	0.967
sqr_000_01493	GdSb	2	-5.186	-5.513	-1.000e-06	0.00316	1.452	0.878
sqr_000_01494	FeV	2	-8.669	-8.71	0.000e+00	0.00466	0.084	0.071
sqr_000_01497	NiRu	2	-7.011	-7.181	-5.000e-06	0.00706	0.459	0.227
sqr_000_01498	NdZn	2	-3.221	-3.224	-3.110e-05	0.0033	0.038	0.033
sqr_000_01501	MoRu	2	-9.718	-10.003	-1.000e-06	0.00425	0.268	0.171
sqr_000_01502	GdHg	2	-2.638	-2.888	-5.300e-06	0.00144	0.312	0.254
sqr_000_01503	DyGa ₂ Li	4	-3.206	-3.507	-7.000e-06	0.00472	0.516	1.445
sqr_000_01508	TbTl	2	-3.203	-3.761	-1.500e-05	0.00555	0.548	0.332
sqr_000_01513	GdSn	2	-4.643	-4.862	0.000e+00	0.00755	0.302	0.442
sqr_000_01519	IrYb	2	-4.861	-5.496	-4.000e-06	0.00068	0.483	0.472
sqr_000_01524	FeRh	2	-7.286	-7.61	-2.000e-06	0.0028	0.358	0.297
sqr_000_01525	AlRu	2	-6.936	-7.115	-1.900e-05	0.00125	0.134	0.058
sqr_000_01527	MnNi	2	-6.875	-7.131	-1.000e-06	0.00567	0.383	0.251
sqr_000_01534	FeGa	2	-5.491	-5.6	-9.000e-06	0.00662	0.187	0.097
sqr_000_01535	MnTi	2	-8.64	-8.645	-8.000e-06	0.00545	0.028	0.03
sqr_000_01537	CdYb	2	-1.479	-1.519	5.000e-07	0.00229	0.157	0.173
sqr_000_01542	FeTb	2	-6.078	-6.122	-2.000e-06	0.00084	0.105	0.072
sqr_000_01545	GdSe	2	-5.544	-5.597	-2.000e-06	0.00347	0.131	0.114
sqr_000_01547	NiPt	2	-5.579	-5.856	-8.000e-06	0.00212	0.383	0.375
sqr_000_01550	RuU	2	-10.12	-10.316	-4.000e-06	0.00136	0.439	0.327
sqr_000_01555	MgNd	2	-3.212	-3.216	-2.000e-07	0.00248	0.056	0.051
sqr_000_01560	CuGaGdTi	4	-4.156	-4.892	0.000e+00	0.0042	0.683	0.57
sqr_000_01561	DySc	2	-5.303	-5.309	3.000e-06	0.00259	0.064	0.067
sqr_000_01563	MnPtSi	3	-6.764	-7.036	1.000e-06	0.00845	0.467	0.467
sqr_000_01564	InRu	2	-5.061	-5.684	0.000e+00	0.00476	0.442	0.281
sqr_000_01571	CdGd	2	-2.958	-2.991	-8.000e-07	0.00283	0.103	0.058

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_01574	NdSi ₂	3	-5.475	-5.753	-1.000e-06	0.00364	0.286	0.23
sqr_000_01575	AuGd	2	-4.703	-4.764	-1.100e-05	0.00137	0.195	0.18
sqr_000_01577	NdPd	2	-5.54	-5.694	-1.500e-05	0.00182	0.218	0.173
sqr_000_01582	BeFe	2	-6.024	-6.029	-5.000e-06	0.00238	0.03	0.023
sqr_000_01584	MnRh	2	-7.628	-8.08	-1.200e-05	0.00348	0.374	0.375
sqr_000_01585	DyPd ₃	4	-5.835	-5.935	-3.500e-05	0.00139	0.175	0.146
sqr_000_01586	AgAlInNd	4	-2.391	-3.645	0.000e+00	0.00725	0.526	0.459
sqr_000_01599	MnRu	2	-8.713	-8.977	-1.700e-05	0.00106	0.299	0.381
sqr_000_01601	GdSb	2	-4.566	-5.269	0.000e+00	0.00392	0.572	0.385
sqr_000_01603	FeRu	2	-8.431	-8.554	1.000e-06	0.00632	0.11	0.122
sqr_000_01608	CdDy	2	-2.935	-2.97	-1.700e-06	0.00218	0.125	0.081
sqr_000_01609	Mg ₂ NdSn	4	-3.269	-3.321	-1.000e-06	0.00405	0.17	0.127
sqr_000_01611	GaGdMnSn	4	-4.935	-5.036	-1.000e-06	0.00397	0.359	0.255
sqr_000_01612	HoYb	2	-2.75	-2.805	-3.610e-05	0.00045	0.18	0.049
sqr_000_01618	CdGd	2	-2.955	-2.991	-4.500e-06	0.00536	0.102	0.089
sqr_000_01619	MgTb	2	-3.071	-3.12	-6.900e-06	0.00102	0.147	0.105
sqr_000_01622	TbZn ₃	4	-1.895	-2.178	-4.000e-07	0.00154	0.336	0.214
sqr_000_01623	TeYb	2	-3.399	-3.816	-7.000e-07	0.00045	0.349	0.289
sqr_000_01626	FeMn ₂ Rh	4	-8.272	-8.288	-1.000e-06	0.00516	0.062	0.926
sqr_000_01630	DyTb	2	-4.037	-4.479	-1.500e-06	0.00158	0.384	0.321
sqr_000_01631	NaNiS ₂	4	-3.573	-4.225	-1.000e-06	0.0069	0.621	0.88
sqr_000_01633	InRu	2	-5.446	-5.748	-2.000e-06	0.0015	0.358	0.313
sqr_000_01635	FeNi	2	-6.193	-6.642	-1.000e-06	0.00407	0.541	0.402
sqr_000_01638	GdZn	2	-3.111	-3.191	3.600e-06	0.00027	0.177	0.105
sqr_000_01642	FeRh	2	-7.464	-7.605	-1.000e-06	0.00735	0.121	0.152
sqr_000_01646	MnRu	2	-8.716	-8.978	-2.000e-06	0.00314	0.346	0.399
sqr_000_01648	RhTb	2	-6.281	-6.751	2.000e-06	0.00056	0.348	0.173
sqr_000_01649	HfRu	2	-9.443	-10.305	-1.000e-06	0.00164	0.445	0.37
sqr_000_01650	RuZn	2	-4.885	-4.981	-1.600e-06	0.00086	0.319	0.321
sqr_000_01652	Nd ₂	2	-4.612	-4.703	-6.000e-07	0.00179	0.422	0.531
sqr_000_01655	CdTb	2	-2.689	-2.992	4.000e-07	0.00143	0.37	0.181
sqr_000_01657	RhTb	2	-6.458	-6.747	1.000e-06	0.00253	0.28	0.117
sqr_000_01659	NiRh	2	-6.221	-6.302	-1.000e-05	0.00831	0.284	0.222
sqr_000_01663	MnZn	2	-4.574	-4.797	-6.400e-06	0.00269	0.505	0.367
sqr_000_01672	CBCoGd	4	-7.031	-7.227	-4.000e-06	0.00515	0.2	0.213
sqr_000_01673	BeRu	2	-6.545	-6.654	0.000e+00	0.00052	0.106	0.038
sqr_000_01675	AlGdRhTi	4	-5.66	-6.159	-5.000e-06	0.00855	0.702	0.35
sqr_000_01679	PdTb	2	-5.751	-5.756	-1.700e-05	0.00162	0.046	0.036
sqr_000_01680	SrYb	2	-1.098	-1.55	-2.000e-06	0.00051	0.655	0.452
sqr_000_01683	BeRu	2	-6.465	-6.677	0.000e+00	0.00289	0.175	0.104
sqr_000_01687	FeNi	2	-6.513	-6.633	-5.000e-06	0.00526	0.281	0.296
sqr_000_01689	DyEu	2	-3.005	-3.011	-4.500e-06	0.00249	0.064	0.033
sqr_000_01692	AuDy	2	-4.752	-4.758	3.000e-07	0.0034	0.04	0.029
sqr_000_01701	FeGa	2	-5.408	-5.597	0.000e+00	0.00169	0.518	0.357
sqr_000_01705	TbZn	2	-3.143	-3.183	-1.600e-06	0.00408	0.125	0.05
sqr_000_01708	TbY	2	-4.875	-5.453	-1.800e-05	0.002	0.437	0.539
sqr_000_01711	GaNd	2	-4.363	-4.369	5.500e-06	0.00178	0.054	0.05
sqr_000_01715	NdNiPt ₂	4	-5.736	-6.2	1.000e-06	0.00457	0.286	0.243
sqr_000_01716	PtRu	2	-7.218	-7.529	-3.000e-06	0.00865	0.428	0.346
sqr_000_01717	Au ₂ DyMn	4	-4.726	-5.05	-2.000e-05	0.00403	0.717	1.566
sqr_000_01718	TbZn	2	-3.144	-3.183	-9.200e-06	0.00151	0.121	0.074
sqr_000_01719	NdSe	2	-5.651	-5.731	-1.300e-05	0.0028	0.214	0.231

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_01720	RuU	2	-9.564	-10.293	-6.000e-06	0.00192	0.553	0.42
sqr_000_01721	GdPd	2	-5.731	-5.75	1.000e-06	0.00127	0.073	0.069
sqr_000_01722	MgYb	2	-1.514	-1.529	2.000e-07	0.00095	0.183	0.232
sqr_000_01728	NdTl	2	-3.552	-3.859	-2.300e-05	0.00156	0.302	0.205
sqr_000_01742	AsTb	2	-5.675	-6.127	-7.000e-06	0.00438	1.306	1.044
sqr_000_01751	FeRh	2	-7.334	-7.602	-1.400e-05	0.00345	0.146	0.216
sqr_000_01753	GdSb	2	-5.122	-5.263	-1.000e-05	0.00067	0.374	0.153
sqr_000_01754	PtRu	2	-7.209	-7.553	0.000e+00	0.00661	0.432	0.353
sqr_000_01757	MnV	2	-9.165	-9.275	1.000e-06	0.00206	0.145	0.14
sqr_000_01760	NiV	2	-7.229	-7.407	-	0.00415	0.177	0.071
					3.205e+00			
sqr_000_01763	CdTb	2	-2.945	-2.979	1.000e-07	0.00263	0.094	0.04
sqr_000_01766	LiTb	2	-3.038	-3.077	0.000e+00	0.00067	0.155	0.064
sqr_000_01769	MgTb	2	-3.046	-3.119	-1.100e-06	0.00028	0.168	0.096
sqr_000_01773	SbYb	2	-3.587	-3.593	4.600e-06	0.00123	0.115	0.123
sqr_000_01776	FeHo	2	-5.004	-6.099	0.000e+00	0.00293	0.947	0.888
sqr_000_01777	RuTa	2	-10.52	-10.815	-1.500e-05	0.00378	0.146	0.191
sqr_000_01780	AgTb	2	-3.647	-3.984	-3.000e-06	0.00509	0.42	0.411
sqr_000_01782	BeNi	2	-5.038	-5.084	-1.000e-06	0.00125	0.143	0.106
sqr_000_01786	NdS	2	-5.649	-6.15	0.000e+00	0.00353	0.424	0.196
sqr_000_01787	GdHo	2	-4.473	-4.524	-1.700e-06	0.00028	0.239	0.148
sqr_000_01790	GdPr	2	-4.151	-4.659	7.000e-07	0.00174	0.501	0.769
sqr_000_01792	AsGd	2	-5.049	-6.171	1.000e-06	0.00254	1.15	1.024
sqr_000_01796	AuGd	2	-4.746	-4.764	-3.000e-07	0.00693	0.101	0.051
sqr_000_01797	SbTb	2	-4.973	-5.467	-1.000e-06	0.0006	1.445	0.531
sqr_000_01799	NiRh	2	-6.212	-6.309	-5.000e-06	0.00591	0.164	0.125
sqr_000_01811	Al ₂ CuTb	4	-3.817	-4.203	1.000e-05	0.004	0.35	0.303
sqr_000_01813	MnMoRh	3	-8.649	-8.976	-3.000e-06	0.00959	0.544	0.261
sqr_000_01814	FeZn	2	-4.3	-4.34	3.500e-06	0.00387	0.133	0.108
sqr_000_01823	DyHg	2	-2.841	-2.853	-6.000e-07	0.00195	0.062	0.044
sqr_000_01824	DyMg	2	-3.064	-3.099	-1.800e-06	0.00068	0.231	0.149
sqr_000_01825	GaNi	2	-4.531	-4.551	1.000e-06	0.00324	0.066	0.048
sqr_000_01829	CoTi	2	-7.743	-7.807	-2.000e-06	0.0028	0.172	0.157
sqr_000_01830	GdSn	2	-4.404	-4.863	-1.000e-06	0.00233	0.501	0.278
sqr_000_01832	Au ₂ GdPd	4	-4.196	-4.795	-7.000e-06	0.00529	0.369	0.252
sqr_000_01838	GdYb	2	-2.608	-2.864	7.000e-07	0.00088	0.362	0.201
sqr_000_01845	AgNd	2	-3.725	-4.004	0.000e+00	0.00097	0.353	0.224
sqr_000_01846	CoZn	2	-3.934	-4.02	-1.500e-06	0.00236	0.13	0.041
sqr_000_01847	CaYb	2	-1.43	-1.674	1.100e-06	0.00054	0.495	0.551
sqr_000_01854	TbTe	2	-4.946	-5.039	-2.000e-06	0.00288	0.293	0.273
sqr_000_01857	GdTe	2	-4.746	-5.09	-1.400e-05	0.00257	0.363	0.191
sqr_000_01860	NdTl	2	-3.855	-3.866	4.000e-06	0.00083	0.139	0.114
sqr_000_01863	HgYb	2	-1.429	-1.477	-4.000e-07	0.00202	0.163	0.119
sqr_000_01864	DyGe	2	-4.665	-5.159	1.000e-06	0.00384	0.68	0.722
sqr_000_01865	DyInYbZn	4	-2.047	-2.795	-1.000e-06	0.00552	1.017	1.693
sqr_000_01869	CdNd	2	-2.984	-3.058	-2.300e-06	0.00808	0.181	0.117
sqr_000_01870	FeRh	2	-7.531	-7.613	-6.000e-06	0.00333	0.125	0.067
sqr_000_01876	NdSn	2	-4.721	-4.96	-8.800e-06	0.00847	0.5	0.313
sqr_000_01877	PtTb	2	-6.274	-6.335	0.000e+00	0.00329	0.268	0.107
sqr_000_01881	FeMn	2	-8.194	-8.528	0.000e+00	0.00334	0.422	0.328
sqr_000_01890	Si ₂ Tb	3	-5.22	-5.671	0.000e+00	0.00394	0.347	0.23
sqr_000_01891	MgTb	2	-3.034	-3.119	-9.200e-06	0.00047	0.215	0.146

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_01893	MgYb	2	-1.489	-1.529	-1.000e-07	0.00034	0.265	0.158
sqr_000_01897	GaGd	2	-4.304	-4.335	8.000e-07	0.0091	0.124	0.106
sqr_000_01898	Al ₂ GdP	4	-4.045	-4.94	-8.000e-06	0.00706	0.717	1.154
sqr_000_01900	GaNd	2	-4.141	-4.373	3.900e-06	0.00064	0.313	0.261
sqr_000_01904	HgTb	2	-2.7	-2.874	4.800e-06	0.00252	0.251	0.147
sqr_000_01905	SeTb	2	-5.557	-5.558	0.000e+00	0.00058	0.019	0.03
sqr_000_01910	GdY	2	-5.154	-5.478	0.000e+00	0.0034	0.44	0.352
sqr_000_01920	MgYb	2	-1.513	-1.526	-4.820e-05	0.0012	0.13	0.084
sqr_000_01924	RuSc	2	-7.927	-8.227	-4.600e-05	0.00206	0.25	0.188
sqr_000_01926	CdNd	2	-2.926	-3.042	-3.720e-05	0.00379	0.194	0.118
sqr_000_01928	TlYb	2	-2.338	-2.341	-9.000e-07	0.00329	0.042	0.04
sqr_000_01929	BrGd	2	-3.895	-3.93	3.000e-07	0.00094	0.192	0.161
sqr_000_01934	CdGd	2	-2.967	-2.999	-8.000e-07	0.00208	0.106	0.086
sqr_000_01937	FeNb	2	-9.211	-9.219	1.300e-05	0.00166	0.076	0.083
sqr_000_01943	CdDy	2	-2.913	-2.963	-2.800e-06	0.00158	0.125	0.092
sqr_000_01945	DyRh	2	-6.027	-6.777	1.000e-06	0.00192	0.457	0.236
sqr_000_01947	Yb ₂	2	-1.278	-1.446	0.000e+00	0.0009	0.364	0.316
sqr_000_01950	MnRu	2	-8.842	-8.976	1.000e-06	0.0008	0.151	0.212
sqr_000_01952	NiRu	2	-7.022	-7.196	-5.000e-06	0.00207	0.347	0.307
sqr_000_01953	FeRu	2	-7.897	-8.546	-6.000e-06	0.00297	0.223	0.17
sqr_000_01954	NdP	2	-6.105	-6.292	-2.000e-06	0.00246	0.463	0.341
sqr_000_01956	DySc	2	-5.161	-5.328	0.000e+00	0.00211	0.297	0.476
sqr_000_01958	CdNd	2	-2.94	-3.059	-3.710e-05	0.00119	0.227	0.183
sqr_000_01961	GaMgMnZn	4	-3.219	-3.367	1.000e-06	0.00755	0.479	0.447
sqr_000_01963	ThYb	2	-4.115	-4.223	9.400e-06	0.00271	0.656	0.852
sqr_000_01965	AgGd	2	-3.975	-3.985	5.000e-07	0.0013	0.089	0.07
sqr_000_01966	AlMnOs	3	-7.699	-8.233	-1.000e-06	0.00684	0.476	0.657
sqr_000_01972	FePt	2	-6.785	-7.061	-5.000e-06	0.00593	0.444	0.298
sqr_000_01975	MgNd	2	-3.166	-3.22	-9.000e-06	0.00106	0.163	0.09
sqr_000_01976	CoMo	2	-8.606	-8.942	-1.000e-06	0.00969	0.168	0.113
sqr_000_01977	CuGd	2	-4.321	-4.395	-5.500e-06	0.0003	0.161	0.148
sqr_000_01978	AgDy	2	-3.953	-3.972	-1.850e-05	0.00088	0.095	0.068
sqr_000_01979	Ga ₂ NdPt	4	-4.406	-4.753	0.000e+00	0.00608	0.316	1.274
sqr_000_01982	AsNd	2	-5.528	-6.186	0.000e+00	0.00037	1.359	1.49
sqr_000_01983	GaRu	2	-5.924	-6.341	-1.200e-05	0.0028	0.256	0.194
sqr_000_01985	NdPr	2	-4.389	-4.708	-9.600e-06	0.0014	0.491	0.696
sqr_000_01987	AgTb	2	-3.931	-3.977	-2.700e-06	0.00254	0.128	0.088
sqr_000_01988	DyZn	2	-3.165	-3.172	-2.200e-06	0.0018	0.065	0.042
sqr_000_01989	IrNi	2	-6.586	-7.116	-2.000e-06	0.00287	0.213	0.139
sqr_000_01990	DyZr	2	-6.169	-6.372	1.000e-06	0.00145	0.443	0.63
sqr_000_01992	RuZr	2	-9.223	-9.523	1.000e-06	0.00023	0.354	0.327
sqr_000_01994	CdGdPd	3	-3.923	-4.1	-5.000e-06	0.00397	0.201	0.207
sqr_000_01996	Ni ₂	2	-5.284	-5.415	0.000e+00	0.00022	0.41	0.436
sqr_000_02000	In ₃ Yb	4	-2.111	-2.629	2.000e-06	0.00368	0.426	0.372
sqr_000_02001	CoPt	2	-6.222	-6.49	-3.000e-06	0.00084	0.309	0.407
sqr_000_02002	GaMn	2	-5.779	-5.805	0.000e+00	0.00222	0.108	0.073
sqr_000_02004	NdSe	2	-5.505	-5.732	-2.300e-05	0.00167	0.346	0.276
sqr_000_02011	NiOs	2	-7.922	-8.143	-3.000e-06	0.00141	0.269	0.373
sqr_000_02012	NiRh	2	-6.027	-6.303	0.000e+00	0.00496	0.184	0.148
sqr_000_02013	CoRu	2	-7.695	-7.963	8.000e-06	0.0044	0.469	0.446
sqr_000_02018	DyZn	2	-3.171	-3.172	-3.200e-06	0.00321	0.016	0.013
sqr_000_02019	LiRu	2	-4.864	-5.127	0.000e+00	0.00308	0.282	0.179

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_02020	BeNi	2	-4.997	-5.083	-6.000e-06	0.00441	0.111	0.083
sqr_000_02021	MgNd	2	-3.172	-3.217	-3.000e-06	0.00321	0.154	0.115
sqr_000_02022	TlYb	2	-2.337	-2.342	0.000e+00	0.00126	0.053	0.049
sqr_000_02024	DyTh	2	-5.723	-5.948	-2.000e-06	0.00173	0.513	0.705
sqr_000_02027	TlYb	2	-2.061	-2.362	-8.750e-05	0.00129	0.493	0.337
sqr_000_02028	AgDyPt ₂	4	-5.427	-5.683	0.000e+00	0.00183	0.222	0.194
sqr_000_02031	SbTb	2	-4.404	-5.496	0.000e+00	0.00118	1.401	0.92
sqr_000_02033	HNiRu	3	-5.383	-5.859	-7.000e-06	0.00505	0.694	1.094
sqr_000_02038	BiTb	2	-4.75	-4.964	6.000e-07	0.0021	0.812	0.546
sqr_000_02044	RuSm	2	-7.037	-7.065	-1.000e-06	0.00575	0.084	0.046
sqr_000_02057	AgYb	2	-2.45	-2.525	-4.100e-06	0.00129	0.22	0.118
sqr_000_02058	CoGeNdZr	4	-6.233	-6.406	-8.000e-06	0.00639	0.503	0.595
sqr_000_02059	GdP	2	-6.109	-6.602	-6.000e-06	0.00104	1.183	1.28
sqr_000_02061	DyZn ₃	4	-2.181	-2.187	3.000e-07	0.00296	0.039	0.032
sqr_000_02065	DyTl	2	-3.662	-3.725	-6.000e-07	0.00225	0.253	0.148
sqr_000_02066	CdTb	2	-2.882	-2.975	-1.000e-07	0.00333	0.164	0.134
sqr_000_02067	MnZn	2	-4.625	-4.79	-8.000e-07	0.00192	0.541	0.318
sqr_000_02072	AlCo	2	-5.985	-5.989	-1.400e-04	0.00752	0.027	0.032
sqr_000_02074	Al ₃ Dy	4	-3.263	-4.356	-1.000e-06	0.00285	0.489	0.429
sqr_000_02080	DyHg	2	-2.831	-2.85	-1.060e-05	0.00112	0.114	0.088
sqr_000_02087	Ge ₂ Mn ₂	4	-6.319	-6.627	-2.000e-06	0.00476	0.556	0.497
sqr_000_02090	AlFeNbRu	4	-8.112	-8.288	-1.000e-06	0.00353	0.228	0.183
sqr_000_02094	BiGd	2	-4.875	-4.957	-1.000e-06	0.0033	0.395	0.195
sqr_000_02100	CdGd	2	-2.979	-2.991	-1.600e-06	0.00237	0.074	0.054
sqr_000_02101	AlNi	2	-5.112	-5.265	-5.000e-06	0.00257	0.374	0.257
sqr_000_02105	NdSb	2	-5.275	-5.599	-4.000e-06	0.00197	1.394	1.199
sqr_000_02108	Co ₂	2	-6.777	-6.842	-2.011e-03	0.00652	0.09	0.059
sqr_000_02115	BiNd	2	-4.988	-5.079	8.000e-06	0.00098	0.426	0.338
sqr_000_02116	FeRu	2	-8.39	-8.564	-3.000e-06	0.00057	0.179	0.252
sqr_000_02119	NiPt	2	-5.534	-5.868	-2.000e-06	0.00605	0.32	0.284
sqr_000_02120	MgYb	2	-1.516	-1.529	-2.900e-06	0.00312	0.173	0.221
sqr_000_02122	GdYb	2	-2.805	-2.873	-1.110e-05	0.0005	0.193	0.087
sqr_000_02128	GdTl	2	-3.768	-3.787	-4.000e-06	0.00161	0.085	0.044
sqr_000_02129	InNd	2	-4.297	-3.699	-5.069e-04	0.00244	0.218	0.222
sqr_000_02140	AgNd	2	-3.973	-3.993	-3.300e-05	0.00134	0.082	0.055
sqr_000_02144	GdTe	2	-4.957	-5.088	-1.000e-06	0.00215	0.213	0.096
sqr_000_02149	NdSn	2	-4.772	-4.954	-3.500e-06	0.00163	0.493	0.387
sqr_000_02152	AsNd	2	-5.772	-6.171	1.800e-05	0.00365	1.299	1.258
sqr_000_02156	CoRh	2	-6.828	-7.007	2.000e-06	0.00602	0.128	0.155
sqr_000_02157	TbTm	2	-4.104	-4.459	7.000e-07	0.00208	0.365	0.663
sqr_000_02160	PuRu	2	-11.014	-11.275	-1.700e-05	0.00178	0.819	0.694
sqr_000_02161	AlliMnN	4	-3.749	-5.912	0.000e+00	0.00687	1.074	1.485
sqr_000_02163	EuYb	2	-1.446	-1.654	2.000e-07	0.00371	0.426	0.269
sqr_000_02167	PbYb	2	-3.043	-3.074	-2.200e-06	0.0032	0.292	0.22
sqr_000_02168	FeGaNdNp	4	30.11	-6.975	0.000e+00	0.00724	0.769	1.206
sqr_000_02169	Fe ₂ GdTi	4	-6.637	-7.084	-1.400e-04	0.00731	0.612	0.578
sqr_000_02170	CaDy	2	-2.981	-3.04	3.400e-06	0.0022	0.188	0.093
sqr_000_02172	GdS	2	-5.847	-6.043	0.000e+00	0.00095	0.345	0.272
sqr_000_02182	NiPt	2	-5.749	-5.861	-4.000e-06	0.00747	0.259	0.228
sqr_000_02184	HfRu	2	-9.878	-10.348	-4.100e-05	0.00421	0.438	0.482
sqr_000_02187	CoNb	2	-8.235	-8.679	-5.800e-05	0.00565	0.442	0.294
sqr_000_02194	CoFePt	3	-6.407	-6.998	0.000e+00	0.00641	0.623	0.784

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_02198	FeNi	2	-6.384	-6.624	-2.000e-06	0.00251	0.332	0.47
sqr_000_02200	PRu	2	-7.035	-7.539	-3.000e-06	0.00085	0.628	0.279
sqr_000_02204	CsNd	2	-1.734	-1.923	3.900e-06	0.00415	0.747	0.555
sqr_000_02205	GdTl	2	-3.507	-3.796	-4.000e-07	0.00099	0.37	0.327
sqr_000_02206	GdNd	2	-4.58	-4.646	-4.690e-05	0.0042	0.286	0.29
sqr_000_02208	NaNd	2	-2.628	-2.637	3.700e-06	0.00374	0.264	0.18
sqr_000_02210	NdZr	2	-6.304	-6.385	-6.900e-05	0.00746	0.556	0.657
sqr_000_02211	RuZr	2	-9.511	-9.525	-1.300e-05	0.00374	0.07	0.079
sqr_000_02219	GdZn	2	-2.935	-3.192	-3.700e-06	0.00499	0.336	0.233
sqr_000_02227	GdTe	2	-4.614	-5.09	-4.000e-06	0.00136	0.442	0.24
sqr_000_02228	RuTm	2	-7.225	-7.23	-1.300e-05	0.00254	0.047	0.042
sqr_000_02229	BeCo	2	-5.67	-5.699	-1.000e-06	0.00382	0.082	0.075
sqr_000_02230	AsDy	2	-5.65	-6.118	-2.000e-06	0.00252	1.251	1.102
sqr_000_02231	DyTl	2	-3.729	-3.729	-5.100e-06	0.00346	0.01	0.014
sqr_000_02236	AcCdYb	3	-2.171	-2.302	3.200e-06	0.0025	0.294	0.325
sqr_000_02237	LuRu	2	-6.288	-7.128	-3.000e-06	0.00328	0.647	0.432
sqr_000_02238	MgRu	2	-4.94	-5.115	0.0000e+00	0.00386	0.205	0.128
sqr_000_02240	GaNd	2	-4.296	-4.372	6.000e-07	0.00388	0.174	0.104
sqr_000_02249	AgGd	2	-3.798	-3.988	7.000e-07	0.0022	0.276	0.201
sqr_000_02254	DyTe	2	-4.373	-5.0	2.000e-06	0.00316	0.524	0.395
sqr_000_02259	BeDySi	3	-5.123	-5.225	0.0000e+00	0.00417	0.178	0.125
sqr_000_02260	CoNi	2	-5.717	-6.069	-3.000e-06	0.00362	0.472	0.321
sqr_000_02263	FeRh	2	-7.56	-7.614	-2.700e-05	0.00574	0.117	0.139
sqr_000_02271	CuDyPd ₂	4	-5.321	-5.323	-3.000e-06	0.00559	0.022	0.025
sqr_000_02273	GaGd	2	-4.312	-4.338	-1.460e-05	0.00197	0.091	0.064
sqr_000_02280	AgYb	2	-2.28	-2.531	-2.100e-06	0.00144	0.422	0.178
sqr_000_02281	TbZn	2	-3.025	-3.181	-5.200e-06	0.00103	0.251	0.112
sqr_000_02282	FeNi	2	-6.326	-6.641	-3.300e-05	0.0052	0.348	0.481
sqr_000_02286	GdPd	2	-5.738	-5.75	-1.100e-05	0.00263	0.054	0.039
sqr_000_02287	NdTl	2	-3.599	-3.875	-1.400e-06	0.00193	0.365	0.25
sqr_000_02288	CdGd	2	-2.993	-2.994	-7.900e-06	0.00196	0.014	0.021
sqr_000_02290	FeNi	2	-6.522	-6.633	0.0000e+00	0.00161	0.261	0.16
sqr_000_02292	AlGd	2	-4.543	-4.564	-4.000e-07	0.00326	0.086	0.071
sqr_000_02293	Dy ₂	2	-3.985	-4.459	1.000e-07	0.00582	0.405	0.716
sqr_000_02302	GdLi	2	-3.058	-3.104	-3.000e-06	0.00386	0.18	0.145
sqr_000_02305	AuGd	2	-4.724	-4.765	-2.400e-06	0.00444	0.11	0.106
sqr_000_02308	NdZn	2	-3.219	-3.223	1.700e-06	0.00201	0.036	0.028
sqr_000_02309	GaRhTb ₂	4	-5.156	-5.485	-1.000e-06	0.00443	0.667	0.568
sqr_000_02311	PTb	2	-5.579	-6.597	0.0000e+00	0.00152	1.297	1.239
sqr_000_02322	FeZn	2	-4.168	-4.326	-2.900e-06	0.00359	0.169	0.101
sqr_000_02333	CdGd	2	-2.818	-3.003	-8.000e-07	0.00296	0.28	0.17
sqr_000_02336	CoNi	2	-5.63	-6.07	-1.000e-06	0.00504	0.392	0.181
sqr_000_02338	SeYb	2	-4.102	-4.558	-6.000e-07	0.00221	1.258	0.969
sqr_000_02343	RhRu	2	-7.328	-8.128	-6.000e-06	0.00382	0.217	0.331
sqr_000_02345	NdRu	2	-6.537	-6.959	-7.000e-05	0.00934	0.55	0.328
sqr_000_02348	Rh ₃ Yb	4	-6.111	-6.135	-6.000e-06	0.00276	0.073	0.045
sqr_000_02349	TbTl	2	-3.751	-3.756	-1.800e-06	0.00178	0.049	0.047
sqr_000_02350	NiPt	2	-5.731	-5.861	-1.100e-05	0.00852	0.139	0.091
sqr_000_02356	CdNd	2	-3.04	-3.055	-6.100e-06	0.00223	0.071	0.049
sqr_000_02358	BeFe	2	-6.003	-6.027	8.000e-06	0.00885	0.06	0.052
sqr_000_02369	MnNi	2	-7.017	-7.137	-2.600e-05	0.00658	0.15	0.173
sqr_000_02373	CoMn	2	-7.863	-7.956	-3.000e-06	0.005	0.112	0.07

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_02377	GdRh	2	-6.518	-6.722	-2.000e-06	0.00391	0.218	0.147
sqr_000_02378	AsNd	2	-5.77	-6.166	-1.000e-06	0.00653	1.283	1.488
sqr_000_02379	GdPd	2	-5.72	-5.75	0.000e+00	0.00346	0.151	0.177
sqr_000_02382	ScTb	2	-5.322	-5.352	-4.000e-06	0.00164	0.448	2.084
sqr_000_02385	NdYb	2	-2.815	-2.993	1.200e-06	0.00112	0.315	0.164
sqr_000_02388	HfRu	2	-10.27	-10.381	-2.400e-05	0.00223	0.118	0.084
sqr_000_02397	AlGd	2	-4.526	-4.564	-1.600e-06	0.00239	0.117	0.081
sqr_000_02400	GdTe	2	-4.526	-5.09	2.000e-06	0.00122	0.495	0.371
sqr_000_02402	DyNi ₂ Pd	4	-5.157	-5.605	3.000e-06	0.00499	0.305	0.315
sqr_000_02406	DyLa	2	-4.197	-4.669	0.000e+00	0.00199	0.448	0.411
sqr_000_02409	DyGdPd	3	-4.285	-5.207	1.000e-06	0.00218	0.771	0.77
sqr_000_02414	NiPt	2	-5.606	-5.853	-3.000e-06	0.00676	0.285	0.428
sqr_000_02420	DyPt	2	-6.518	-6.53	1.000e-06	0.00349	0.055	0.02
sqr_000_02426	MnPd	2	-6.544	-6.81	-1.000e-06	0.00101	0.43	0.309
sqr_000_02429	MgNd	2	-3.173	-3.22	-2.640e-05	0.00047	0.224	0.138
sqr_000_02433	SeYb	2	-4.113	-4.262	-6.300e-06	0.00322	0.254	0.149
sqr_000_02436	GdRh	2	-6.354	-6.729	-2.100e-05	0.00301	0.33	0.127
sqr_000_02439	MgYb	2	-1.516	-1.529	-2.700e-06	0.00126	0.174	0.105
sqr_000_02444	AgGd	2	-3.948	-3.983	-3.000e-06	0.00179	0.132	0.073
sqr_000_02451	NaYb	2	-1.254	-1.291	-4.000e-06	0.00142	0.212	0.21
sqr_000_02452	RhTb	2	-6.288	-6.753	0.000e+00	0.00279	0.35	0.199
sqr_000_02456	Gd ₂ Se ₂	4	-5.641	-5.731	-3.000e-06	0.00271	0.221	0.256
sqr_000_02457	GdMg	2	-3.117	-3.142	-1.146e-04	0.00182	0.279	0.218
sqr_000_02461	RuV	2	-9.293	-9.342	-3.400e-05	0.00244	0.08	0.053
sqr_000_02463	TbZn	2	-2.935	-3.182	1.400e-06	0.00126	0.323	0.198
sqr_000_02467	CeGd	2	-4.793	-5.15	2.000e-06	0.00591	0.584	0.68
sqr_000_02470	AgYb	2	-2.452	-2.525	8.000e-07	0.001	0.218	0.093
sqr_000_02472	AgYb	2	-2.447	-2.525	8.200e-06	0.00487	0.226	0.178
sqr_000_02481	CaYb	2	-1.447	-1.675	3.700e-06	0.00043	0.479	0.448
sqr_000_02486	RhTb	2	-6.701	-6.748	-2.200e-05	0.00773	0.101	0.045
sqr_000_02489	CuNTb ₂	4	-5.862	-6.021	-1.200e-05	0.00851	0.254	0.276
sqr_000_02490	CdYb	2	-1.491	-1.519	-4.000e-07	0.00264	0.119	0.065
sqr_000_02504	AgTb	2	-3.926	-3.977	-5.220e-05	0.00172	0.14	0.085
sqr_000_02505	SbYb	2	-3.589	-3.593	-1.600e-06	0.00032	0.041	0.04
sqr_000_02508	SYb	2	-4.045	-4.729	-1.620e-05	0.00615	0.578	0.352
sqr_000_02509	FeTi	2	-8.407	-8.452	-4.000e-06	0.00102	0.082	0.063
sqr_000_02513	CoOs	2	-8.788	-8.944	0.000e+00	0.0071	0.168	0.135
sqr_000_02515	MgTb	2	-3.084	-3.122	-1.500e-06	0.00132	0.148	0.035
sqr_000_02516	AlFe	2	-6.055	-6.3	-4.000e-06	0.00252	0.491	0.482
sqr_000_02524	DyMg	2	-3.001	-3.098	-1.180e-05	0.00037	0.195	0.144
sqr_000_02526	AuCoGdMg	4	-4.045	-4.369	-1.000e-05	0.00761	0.933	1.864
sqr_000_02528	GdMg	2	-3.065	-3.14	-1.400e-06	0.0007	0.173	0.091
sqr_000_02529	MoNi	2	-8.184	-8.19	0.000e+00	0.00355	0.038	0.046
sqr_000_02535	NiTc	2	-7.596	-7.866	-6.000e-06	0.00685	0.182	0.131
sqr_000_02536	CoIr	2	-7.554	-7.88	-1.000e-06	0.00512	0.303	0.274
sqr_000_02542	CoRu	2	-7.691	-7.946	-1.000e-06	0.00493	0.463	0.312
sqr_000_02545	DyZn	2	-3.17	-3.171	-2.300e-06	0.00138	0.029	0.027
sqr_000_02552	FeRu	2	-8.327	-8.564	0.000e+00	0.00038	0.208	0.327
sqr_000_02555	Gd ₂	2	-4.221	-4.544	-2.730e-05	0.00474	0.415	0.496
sqr_000_02563	SnTb	2	-4.638	-4.84	-1.180e-05	0.00526	0.294	0.329
sqr_000_02565	InRu	2	-5.608	-5.76	-2.000e-06	0.00536	0.274	0.251
sqr_000_02566	AgGdPt ₂	4	-5.233	-5.659	0.000e+00	0.00364	0.274	0.259

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_02568	MnNi	2	-7.042	-7.134	0.000e+00	0.00255	0.141	0.11
sqr_000_02579	PdYb	2	-3.916	-4.203	-4.400e-06	0.00071	0.364	0.26
sqr_000_02582	MnPd	2	-6.537	-6.808	-2.000e-06	0.00454	0.477	0.38
sqr_000_02585	TbZr	2	-6.132	-6.356	1.000e-06	0.00193	0.43	0.451
sqr_000_02588	MgTb	2	-3.108	-3.122	-5.200e-06	0.00051	0.083	0.047
sqr_000_02589	CdNd	2	-3.041	-3.049	-3.400e-06	0.00314	0.063	0.05
sqr_000_02593	NdSb	2	-5.292	-5.591	0.000e+00	0.00241	1.417	0.539
sqr_000_02596	NiRu	2	-7.14	-7.201	0.000e+00	0.00733	0.189	0.098
sqr_000_02598	PtTb	2	-6.394	-6.527	0.000e+00	0.00094	0.17	0.077
sqr_000_02602	MnNi	2	-7.039	-7.128	-1.000e-06	0.0028	0.163	0.113
sqr_000_02604	LiMn	2	-4.383	-5.141	-1.700e-05	0.00794	1.014	0.896
sqr_000_02605	RuTm	2	-7.184	-7.23	-4.000e-05	0.00309	0.101	0.083
sqr_000_02608	AsNd	2	-5.775	-6.17	-1.000e-06	0.00169	1.268	1.166
sqr_000_02611	DyGe	2	-5.186	-5.222	1.000e-06	0.00157	0.506	0.428
sqr_000_02616	CBRu	3	-7.134	-8.055	0.000e+00	0.00401	0.722	0.621
sqr_000_02617	HgNd	2	-2.914	-2.919	-3.230e-05	0.00156	0.053	0.043
sqr_000_02620	SnTb	2	-4.606	-4.836	-9.700e-06	0.00222	0.482	0.353
sqr_000_02622	GdTl	2	-3.758	-3.788	-9.900e-06	0.00224	0.104	0.063
sqr_000_02626	PdRu	2	-6.652	-6.947	-1.000e-06	0.0051	0.556	1.821
sqr_000_02627	AsTb	2	-5.507	-6.14	0.000e+00	0.00055	1.331	1.04
sqr_000_02629	AgDy	2	-3.944	-3.971	-4.000e-07	0.00241	0.095	0.035
sqr_000_02631	AgAuDy	3	-4.076	-4.131	1.000e-06	0.00359	0.233	0.213
sqr_000_02632	NdTl	2	-3.72	-3.876	-5.600e-06	0.00195	0.267	0.188
sqr_000_02643	NdTi	2	-5.889	-5.89	-2.070e-04	0.00533	0.012	0.011
sqr_000_02647	MnNi	2	-7.046	-7.126	-1.100e-05	0.00425	0.165	0.207
sqr_000_02648	IrMn	2	-8.652	-9.025	0.000e+00	0.00049	0.183	0.209
sqr_000_02651	FeRu	2	-8.48	-8.563	-5.000e-06	0.00034	0.129	0.132
sqr_000_02656	CdTb	2	-2.827	-2.987	-1.300e-06	0.00041	0.255	0.154
sqr_000_02672	SbYb	2	-3.59	-3.592	-3.290e-05	0.00855	0.063	0.069
sqr_000_02678	AuRu	2	-5.43	-5.724	-3.200e-05	0.00434	0.329	0.432
sqr_000_02685	CaGd	2	-2.904	-3.091	-1.050e-05	0.00029	0.313	0.216
sqr_000_02689	MnRh	2	-7.679	-8.079	-4.000e-06	0.00473	0.256	0.376
sqr_000_02691	NdSb	2	-5.275	-5.598	-3.000e-06	0.0011	1.402	1.327
sqr_000_02692	GdIn	2	-3.998	-4.065	-5.700e-06	0.0075	0.145	0.081
sqr_000_02693	AlNd	2	-4.33	-4.584	-2.500e-06	0.00145	0.336	0.13
sqr_000_02694	CdNd	2	-3.011	-3.057	-1.400e-06	0.00103	0.144	0.04
sqr_000_02702	DyPt	2	-6.517	-6.53	0.000e+00	0.00522	0.061	0.039
sqr_000_02711	MgTb	2	-3.021	-3.119	-2.100e-05	0.00188	0.202	0.079
sqr_000_02714	AgNi	2	-3.412	-3.797	-4.400e-06	0.00848	0.203	0.127
sqr_000_02715	CdYb	2	-1.416	-1.521	-6.000e-07	0.00324	0.271	0.127
sqr_000_02716	TeYb	2	-3.665	-3.965	-2.900e-06	0.0012	1.381	0.982
sqr_000_02717	MgNd	2	-3.215	-3.216	-2.000e-06	0.00056	0.028	0.022
sqr_000_02718	MnRu	2	-8.733	-8.984	-3.000e-06	0.00472	0.395	0.388
sqr_000_02719	NdSm	2	-4.184	-4.674	-1.000e-07	0.00358	0.449	0.448
sqr_000_02723	AgTb	2	-3.733	-3.983	-4.100e-06	0.0019	0.323	0.274
sqr_000_02725	BiTb	2	-4.824	-4.924	-3.100e-06	0.00209	0.338	0.121
sqr_000_02728	GdTb	2	-4.003	-4.514	-2.400e-06	0.00293	0.409	0.686
sqr_000_02731	Al ₂ MgTb	4	-3.654	-3.721	0.000e+00	0.00289	0.171	0.15
sqr_000_02735	AgNd	2	-3.886	-3.999	1.060e-05	0.00263	0.213	0.083
sqr_000_02737	NiRh	2	-6.109	-6.311	-1.400e-05	0.00187	0.417	0.279
sqr_000_02738	MgTb	2	-3.121	-3.122	-3.400e-06	0.00066	0.021	0.014
sqr_000_02739	GdV	2	-6.08	-6.114	-1.200e-05	0.00144	0.101	0.069

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_02740	NdRh	2	-6.405	-6.602	-3.000e-06	0.00426	0.227	0.22
sqr_000_02747	GdSb	2	-4.851	-5.268	0.000e+00	0.00746	0.435	0.304
sqr_000_02750	InTb	2	-3.962	-4.055	-4.810e-05	0.0061	0.188	0.121
sqr_000_02752	GdSn	2	-4.689	-4.868	-4.000e-06	0.00512	0.314	0.372
sqr_000_02754	FeZn	2	-4.312	-4.34	4.100e-06	0.00268	0.117	0.123
sqr_000_02759	AgDy	2	-3.957	-3.971	-3.000e-07	0.00217	0.078	0.062
sqr_000_02760	TeYb	2	-3.669	-3.963	-1.080e-05	0.00162	1.436	0.435
sqr_000_02762	FeRh	2	-7.557	-7.61	0.000e+00	0.00143	0.081	0.074
sqr_000_02763	MnPt	2	-6.983	-7.549	-1.300e-05	0.00487	0.459	0.462
sqr_000_02772	AlTb	2	-4.357	-4.554	-5.000e-07	0.0003	0.277	0.215
sqr_000_02776	GdSiYb	3	-3.397	-4.044	-4.000e-06	0.00177	0.433	0.559
sqr_000_02777	SbYb	2	-3.569	-3.593	-5.500e-06	0.00455	0.155	0.091
sqr_000_02779	DyMg	2	-2.985	-3.098	4.000e-07	0.00044	0.209	0.134
sqr_000_02784	MgNd	2	-3.198	-3.216	5.000e-07	0.00037	0.098	0.065
sqr_000_02789	TlYb	2	-2.335	-2.342	-2.000e-07	0.00206	0.064	0.064
sqr_000_02791	GdIn	2	-4.037	-4.001	-3.350e-05	0.00916	0.246	0.106
sqr_000_02792	TbZn	2	-3.181	-3.182	-2.800e-06	0.00493	0.012	0.009
sqr_000_02794	TlYb	2	-2.177	-2.364	1.500e-06	0.00389	0.368	0.259
sqr_000_02797	DyZn	2	-3.121	-3.172	-2.570e-05	0.00108	0.138	0.073
sqr_000_02798	GdLi	2	-3.089	-3.101	-4.800e-06	0.00108	0.094	0.07
sqr_000_02799	AuGd	2	-4.485	-4.771	-2.000e-07	0.00347	0.326	0.246
sqr_000_02802	PdTb	2	-5.726	-5.757	-6.500e-05	0.00317	0.094	0.057
sqr_000_02803	FeIr	2	-8.318	-8.526	1.000e-06	0.00128	0.217	0.135
sqr_000_02804	NdRu	2	-6.309	-6.972	1.000e-06	0.00148	0.284	0.169
sqr_000_02807	AgDyGaNi	4	-3.961	-4.181	-2.000e-06	0.00464	0.436	1.557
sqr_000_02809	MgNd	2	-3.175	-3.217	-3.200e-06	0.00037	0.153	0.081
sqr_000_02811	BiYb	2	-3.402	-3.414	2.800e-06	0.00433	0.09	0.059
sqr_000_02815	HMn	2	-4.984	-6.226	-3.000e-06	0.00466	0.801	1.837
sqr_000_02816	RuZr	2	-9.51	-9.524	0.000e+00	0.00604	0.073	0.068
sqr_000_02818	PrYb	2	-2.861	-3.015	-3.250e-05	0.00052	0.295	0.219
sqr_000_02820	GdPr	2	-4.607	-4.656	4.700e-06	0.0043	0.232	0.229
sqr_000_02823	Au ₂ TiYb	4	-3.933	-4.485	-1.200e-05	0.00628	0.906	0.558
sqr_000_02824	HgYb	2	-1.272	-1.486	-2.600e-06	0.00063	0.391	0.255
sqr_000_02825	CdCuDy	3	-3.139	-3.167	-6.000e-07	0.00304	0.219	0.246
sqr_000_02826	TlYb	2	-2.251	-2.351	2.300e-06	0.00317	0.258	0.159
sqr_000_02827	CuHgNdZr	4	-3.251	-4.322	-2.000e-06	0.0053	0.808	0.724
sqr_000_02829	NiTi	2	-6.983	-7.003	-4.000e-06	0.00389	0.092	0.066
sqr_000_02830	DyY	2	-4.988	-5.446	1.000e-06	0.00156	0.403	0.774
sqr_000_02832	AuNd	2	-4.745	-4.751	-2.400e-06	0.00065	0.044	0.016
sqr_000_02835	DyLi	2	-3.014	-3.065	7.000e-07	0.0019	0.171	0.05
sqr_000_02838	CdTb	2	-2.935	-2.982	1.000e-07	0.00331	0.315	0.359
sqr_000_02839	GaTb	2	-4.208	-4.328	-5.730e-05	0.00031	0.217	0.151
sqr_000_02841	AlCo	2	-5.545	-5.994	0.000e+00	0.00531	0.299	0.118
sqr_000_02845	NdRh	2	-6.176	-6.612	-1.000e-06	0.00355	0.36	0.219
sqr_000_02846	NiV	2	-7.295	-7.409	-2.000e-06	0.00566	0.171	0.175
sqr_000_02855	GdYb	2	-2.809	-2.873	-1.750e-05	0.00281	0.188	0.156
sqr_000_02856	AlFe	2	-6.007	-6.3	-3.000e-06	0.005	0.538	0.66
sqr_000_02857	FeTcZn	3	-6.153	-6.508	-1.000e-06	0.00235	0.533	0.457
sqr_000_02858	Se ₂ ThYb	4	-5.388	-5.718	-4.000e-06	0.00455	0.482	0.448
sqr_000_02861	FePt	2	-6.982	-7.062	-1.500e-05	0.00519	0.12	0.104
sqr_000_02862	EuYb	2	-1.402	-1.652	-1.400e-06	0.00163	0.468	0.32
sqr_000_02866	AlRu	2	-7.107	-7.129	-4.000e-06	0.00015	0.077	0.057

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_02867	PdYb	2	-3.916	-4.204	-4.000e-07	0.00093	0.362	0.287
sqr_000_02869	NdTl	2	-3.393	-3.878	1.800e-06	0.002	0.514	0.431
sqr_000_02870	Dy ₂	2	-4.087	-4.466	6.000e-07	0.00311	0.412	0.614
sqr_000_02871	MnTi	2	-8.317	-8.633	-2.200e-05	0.00339	0.279	0.203
sqr_000_02873	PdTb	2	-5.75	-5.756	-3.000e-06	0.00134	0.071	0.04
sqr_000_02878	CaYb	2	-1.404	-1.664	-9.240e-05	0.00124	0.445	0.336
sqr_000_02887	PbTb	2	-4.599	-4.516	-1.000e-07	0.0063	0.497	0.352
sqr_000_02889	Ni ₂	2	-5.153	-5.421	-1.000e-06	0.00281	0.312	0.294
sqr_000_02891	NdSc	2	-5.383	-5.424	0.000e+00	0.00022	0.321	0.49
sqr_000_02893	NiV	2	-7.236	-7.409	2.000e-06	0.0046	0.318	0.277
sqr_000_02898	CdNd	2	-3.044	-3.054	5.900e-06	0.00235	0.074	0.042
sqr_000_02899	GdMg	2	-3.128	-3.14	-6.800e-06	0.00036	0.082	0.069
sqr_000_02900	AlRu	2	-7.084	-7.13	-4.000e-06	0.00082	0.11	0.054
sqr_000_02904	MnTi	2	-8.523	-8.633	-3.400e-05	0.00425	0.115	0.078
sqr_000_02907	MnZn	2	-4.308	-4.799	-2.000e-06	0.0013	0.591	0.592
sqr_000_02909	Be ₃ Mn	4	-3.786	-5.073	0.000e+00	0.00294	0.451	0.305
sqr_000_02914	DyTb	2	-4.287	-4.509	-2.200e-06	0.00017	0.3	0.385
sqr_000_02921	DySm	2	-4.114	-4.569	-3.000e-06	0.0035	0.42	0.348
sqr_000_02922	DyTb	2	-4.476	-4.526	-3.000e-07	0.0019	0.276	0.336
sqr_000_02928	AgTb	2	-3.962	-3.978	-2.000e-07	0.00176	0.071	0.055
sqr_000_02929	DyHf	2	-6.766	-7.017	-1.000e-06	0.00052	0.534	0.654
sqr_000_02930	CoPt	2	-5.984	-6.484	2.000e-06	0.00588	0.236	0.27
sqr_000_02932	NdRh ₂ Ru	4	-7.006	-7.088	-1.000e-06	0.00394	0.282	0.22
sqr_000_02935	GdP	2	-6.037	-6.597	-1.000e-06	0.00616	1.316	1.511
sqr_000_02938	FeMn	2	-8.445	-8.527	-6.000e-06	0.00117	0.194	0.136
sqr_000_02943	NdTl	2	-3.666	-3.878	4.000e-07	0.00199	0.312	0.226
sqr_000_02947	TeYb	2	-3.674	-3.675	-1.300e-06	0.00226	0.022	0.007
sqr_000_02949	MgTb	2	-3.023	-3.119	3.400e-06	0.00069	0.193	0.137
sqr_000_02954	SrYb	2	-1.331	-1.517	-8.000e-07	0.00415	0.405	0.303
sqr_000_02961	MgTb	2	-3.046	-3.119	-5.600e-06	0.00026	0.176	0.108
sqr_000_02966	MnPt	2	-7.417	-7.551	-7.000e-06	0.00408	0.187	0.151
sqr_000_02970	CdDy	2	-2.956	-2.964	-4.300e-06	0.00407	0.051	0.026
sqr_000_02971	NdPt	2	-6.396	-6.439	1.000e-06	0.00244	0.101	0.065
sqr_000_02972	CoMn	2	-7.809	-7.955	-2.500e-05	0.00581	0.166	0.124
sqr_000_02973	SrYb	2	-1.288	-1.513	-3.660e-05	0.00166	0.453	0.38
sqr_000_02976	TlYb	2	-2.338	-2.341	-3.000e-07	0.00058	0.048	0.046
sqr_000_02977	TbTl	2	-3.658	-3.767	-5.690e-05	0.00163	0.205	0.114
sqr_000_02982	RuV	2	-9.326	-9.336	-8.000e-06	0.00317	0.076	0.07
sqr_000_02983	PdRu	2	-6.373	-6.944	-6.000e-06	0.00239	0.589	0.46
sqr_000_02984	GdMg	2	-3.089	-3.14	-6.200e-06	0.00055	0.143	0.132
sqr_000_02992	CdGd	2	-2.928	-2.989	-7.200e-06	0.001	0.144	0.056
sqr_000_03000	Ga ₂ TiYb	4	-3.867	-4.05	-1.000e-06	0.00419	0.923	1.792
sqr_000_03001	SnYb	2	-3.26	-3.342	1.600e-06	0.00594	0.502	0.235
sqr_000_03004	TbTl	2	-3.748	-3.757	-6.200e-06	0.00252	0.08	0.075
sqr_000_03008	DyMg	2	-3.07	-3.1	-1.800e-06	0.00134	0.301	0.308
sqr_000_03010	AgGa ₂ Yb	4	-2.54	-2.809	0.000e+00	0.00602	0.327	1.142
sqr_000_03012	BeNi	2	-5.055	-5.082	2.000e-06	0.00248	0.06	0.039
sqr_000_03014	GdHg	2	-2.866	-2.876	-1.000e-07	0.00367	0.056	0.062
sqr_000_03016	TbTc	2	-7.134	-7.205	2.000e-06	0.0022	0.123	0.079
sqr_000_03019	AgNi ₂ Tb	4	-4.509	-4.735	-7.000e-06	0.00756	0.238	0.169
sqr_000_03020	NdTl	2	-3.852	-3.87	1.200e-06	0.00371	0.127	0.101
sqr_000_03023	NbSi ₂ Tb	4	-6.794	-7.016	-3.000e-06	0.00392	0.197	0.172

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_03026	Ru ₂	2	-8.976	-9.135	0.000e+00	0.00237	0.182	0.153
sqr_000_03027	RhSiTb ₂	4	-4.313	-5.88	-1.800e-05	0.00988	0.524	1.131
sqr_000_03028	GdZn	2	-3.189	-3.192	-1.100e-06	0.00473	0.036	0.035
sqr_000_03029	GdY	2	-5.039	-5.48	3.000e-06	0.00149	0.426	0.505
sqr_000_03030	GdRh	2	-6.651	-6.729	-3.600e-05	0.00661	0.131	0.069
sqr_000_03034	HgNd	2	-2.897	-2.917	-1.580e-05	0.00311	0.081	0.067
sqr_000_03043	HNi	2	-3.886	-4.443	-3.000e-07	0.00346	0.761	0.616
sqr_000_03046	GdS	2	-6.045	-6.215	0.000e+00	0.00395	0.225	0.08
sqr_000_03047	MnMo	2	-9.184	-9.78	-1.600e-05	0.00583	0.383	0.235
sqr_000_03049	ScTb	2	-5.324	-5.328	-3.000e-06	0.00199	0.052	0.034
sqr_000_03052	CuDy	2	-4.376	-4.395	-3.800e-06	0.00181	0.112	0.104
sqr_000_03054	DyPt	2	-6.466	-6.532	-3.000e-06	0.00463	0.116	0.068
sqr_000_03055	AgYb	2	-2.454	-2.525	-1.060e-05	0.00097	0.213	0.175
sqr_000_03059	FeV	2	-8.575	-8.709	0.000e+00	0.00264	0.283	0.227
sqr_000_03062	GaRu	2	-5.985	-6.345	-1.000e-05	0.00271	0.24	0.127
sqr_000_03064	TbYb	2	-2.826	-2.852	-2.800e-06	0.00056	0.147	0.064
sqr_000_03067	DyNd	2	-4.152	-4.612	-8.600e-06	0.00143	0.509	0.617
sqr_000_03069	DyMg	2	-3.059	-3.104	-3.240e-05	0.00236	0.147	0.068
sqr_000_03071	MnRu	2	-8.965	-8.989	-5.000e-06	0.0099	0.069	0.058
sqr_000_03075	RuV	2	-9.146	-9.322	0.000e+00	0.00399	0.141	0.087
sqr_000_03076	SbTb	2	-5.172	-5.486	-1.000e-06	0.00162	1.387	1.581
sqr_000_03079	MgYb	2	-1.52	-1.529	1.000e-07	0.00241	0.173	0.161
sqr_000_03083	TbTl	2	-3.618	-3.751	-1.540e-05	0.00058	0.199	0.103
sqr_000_03085	MnNi ₃	4	-5.963	-6.292	-2.000e-05	0.00458	0.523	1.276
sqr_000_03086	FeRh	2	-7.255	-7.614	5.000e-06	0.00247	0.451	0.376
sqr_000_03087	AgDy ₂ Ni	4	-4.616	-4.683	0.000e+00	0.00228	0.335	0.271
sqr_000_03088	GdSe	2	-5.482	-5.6	0.000e+00	0.0023	0.324	0.296
sqr_000_03094	Ag ₂ Nd	3	-3.627	-3.657	1.000e-06	0.00191	0.163	0.104
sqr_000_03097	In ₂ Yb	3	-2.316	-2.62	-7.600e-06	0.00486	0.554	0.37
sqr_000_03101	BeFe	2	-6.009	-6.028	-2.000e-06	0.00069	0.07	0.063
sqr_000_03103	AsGd	2	-5.69	-6.145	-4.000e-06	0.00224	1.347	0.566
sqr_000_03113	CoTm	2	-5.946	-5.957	1.000e-06	0.00198	0.048	0.032
sqr_000_03114	CdTb	2	-2.845	-2.973	2.000e-07	0.00122	0.192	0.14
sqr_000_03117	NdY	2	-5.446	-5.552	-2.000e-06	0.00226	0.574	0.659
sqr_000_03118	CdYb	2	-1.442	-1.521	-2.400e-06	0.00055	0.248	0.067
sqr_000_03120	NdTl	2	-3.867	-3.868	-2.630e-05	0.00275	0.021	0.016
sqr_000_03124	AgGd	2	-3.979	-3.984	3.000e-07	0.00111	0.058	0.039
sqr_000_03128	TbZn	2	-2.834	-3.182	-6.800e-06	0.00076	0.399	0.303
sqr_000_03131	Ni ₂ PtRu	4	-6.111	-6.542	-3.900e-05	0.00665	0.197	0.181
sqr_000_03135	DyGd	2	-4.011	-4.5	-1.800e-06	0.00592	0.403	0.784
sqr_000_03138	FeRu	2	-8.174	-8.549	1.000e-06	0.0025	0.454	0.371
sqr_000_03139	DyZr	2	-6.134	-6.362	1.000e-06	0.0044	0.436	0.343
sqr_000_03141	NdRu	2	-6.945	-7.008	-1.000e-06	0.00156	0.119	0.093
sqr_000_03145	MnPd	2	-6.729	-6.81	-7.000e-06	0.00589	0.146	0.148
sqr_000_03151	CoZn	2	-3.794	-4.007	-1.600e-06	0.00108	0.686	0.928
sqr_000_03152	GaGeInTb	4	-3.832	-3.908	-1.600e-05	0.00767	0.334	0.31
sqr_000_03159	DyGd	2	-4.072	-4.507	-4.260e-05	0.00249	0.385	0.769
sqr_000_03161	CoTm	2	-5.836	-5.955	-1.000e-06	0.00359	0.149	0.096
sqr_000_03164	Yb ₂	2	-1.298	-1.447	-7.000e-06	0.00162	0.344	0.202
sqr_000_03173	DyLu	2	-4.102	-4.417	-9.100e-06	0.00202	0.394	0.324
sqr_000_03174	NbNi	2	-7.935	-7.997	-2.300e-05	0.00706	0.138	0.064
sqr_000_03175	GeNdTb ₂	4	-4.55	-4.829	-2.000e-06	0.00592	0.285	0.303

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_03179	GdPd	2	-5.351	-5.737	-9.000e-06	0.00113	0.351	0.151
sqr_000_03180	AuTb	2	-4.746	-4.763	7.000e-07	0.00442	0.103	0.109
sqr_000_03181	AlNi	2	-4.943	-5.262	-3.300e-05	0.00455	0.333	0.231
sqr_000_03196	SeTb	2	-5.379	-5.556	0.000e+00	0.00312	0.234	0.156
sqr_000_03198	FeIr	2	-8.006	-8.522	-2.000e-06	0.00743	0.185	0.323
sqr_000_03203	SnTb	2	-4.628	-4.837	-1.190e-05	0.00167	0.318	0.389
sqr_000_03204	AgYb	2	-2.26	-2.532	8.100e-06	0.00116	0.444	0.294
sqr_000_03207	SnTb	2	-4.596	-4.808	-1.570e-05	0.00576	0.276	0.263
sqr_000_03210	DyLi	2	-2.946	-3.065	-2.500e-06	0.00036	0.276	0.109
sqr_000_03214	RuZn	2	-4.81	-5.003	0.000e+00	0.00279	0.176	0.131
sqr_000_03224	AsTbY ₂	4	-5.119	-6.039	1.000e-06	0.00206	0.513	1.2
sqr_000_03228	NbRu	2	-9.802	-9.906	-3.000e-06	0.00244	0.141	0.077
sqr_000_03231	AuTb	2	-4.757	-4.763	-7.300e-06	0.0043	0.059	0.071
sqr_000_03232	RhTb	2	-6.695	-6.748	-2.400e-05	0.00772	0.113	0.055
sqr_000_03234	GdTe	2	-4.979	-5.084	-4.000e-06	0.00166	0.156	0.068
sqr_000_03237	GdYb	2	-2.804	-2.873	-3.000e-07	0.00029	0.195	0.166
sqr_000_03238	DySn	2	-4.493	-4.819	2.400e-06	0.00098	0.481	0.423
sqr_000_03242	FeNi	2	-6.349	-6.629	0.000e+00	0.00559	0.353	0.494
sqr_000_03247	DyLu	2	-4.023	-4.409	2.000e-07	0.00523	0.367	0.636
sqr_000_03248	RuV	2	-9.306	-9.331	-5.800e-05	0.00516	0.054	0.013
sqr_000_03249	MgYb	2	-1.514	-1.529	-3.300e-06	0.00135	0.184	0.26
sqr_000_03250	GdMg	2	-3.095	-3.14	0.000e+00	0.00179	0.168	0.1
sqr_000_03255	CoRu	2	-7.796	-7.951	2.000e-06	0.00727	0.211	0.16
sqr_000_03256	NiPd	2	-5.263	-5.279	-1.900e-05	0.00402	0.142	0.112
sqr_000_03258	RuZn	2	-4.716	-5.004	-1.000e-06	0.004	0.218	0.116
sqr_000_03259	RuZr	2	-8.804	-9.476	-1.000e-06	0.00427	0.381	0.201
sqr_000_03260	GdTe	2	-4.428	-5.09	0.000e+00	0.00098	0.544	0.283
sqr_000_03261	PtRu	2	-7.263	-7.552	0.000e+00	0.00616	0.431	0.277
sqr_000_03263	CoTa	2	-8.792	-9.538	-1.700e-05	0.00802	0.251	0.166
sqr_000_03264	CoMn	2	-7.8	-7.959	-5.000e-06	0.00151	0.113	0.059
sqr_000_03265	MgYb	2	-1.517	-1.529	-1.320e-05	0.00164	0.165	0.163
sqr_000_03266	CuGd	2	-4.12	-4.397	-1.900e-06	0.00534	0.326	0.171
sqr_000_03267	MgYb	2	-1.506	-1.526	-8.300e-06	9e-05	0.154	0.136
sqr_000_03268	Ni ₂	2	-5.192	-5.407	-2.400e-05	0.00457	0.193	0.28
sqr_000_03273	MnPt	2	-7.293	-7.544	-1.000e-06	0.00671	0.157	0.186
sqr_000_03275	Ga ₂ GdZn	4	-2.294	-3.188	-2.200e-05	0.00528	0.838	0.447
sqr_000_03280	DyGa	2	-4.277	-4.304	-1.500e-06	0.00048	0.12	0.096
sqr_000_03282	CoPt	2	-6.236	-6.488	-1.900e-05	0.00467	0.223	0.174
sqr_000_03284	NdZn	2	-3.221	-3.224	-1.600e-06	0.00102	0.035	0.032
sqr_000_03286	MnTc	2	-9.429	-9.562	-2.400e-05	0.00257	0.299	0.264
sqr_000_03289	MgRu	2	-5.072	-5.112	-1.000e-06	0.00036	0.097	0.099
sqr_000_03290	MgTb	2	-3.077	-3.122	-2.100e-06	0.00216	0.188	0.159
sqr_000_03291	FePt	2	-6.863	-7.061	-4.000e-06	0.00662	0.156	0.111
sqr_000_03293	HgYb	2	-1.43	-1.476	-7.000e-06	0.0032	0.161	0.134
sqr_000_03296	GdTb	2	-4.064	-4.515	5.000e-07	0.00114	0.383	0.37
sqr_000_03298	AuYb	2	-3.148	-3.322	4.800e-06	0.00352	0.283	0.156
sqr_000_03302	AgTb	2	-3.938	-3.976	6.000e-07	0.00167	0.113	0.065
sqr_000_03305	FeNi	2	-6.393	-6.636	-2.000e-06	0.00114	0.284	0.252
sqr_000_03307	CoMn	2	-7.849	-7.957	-2.400e-05	0.00604	0.122	0.087
sqr_000_03313	FeZn	2	-3.701	-4.327	-6.300e-06	0.00334	0.406	0.282
sqr_000_03318	Au ₂ Nd	3	-4.44	-4.508	1.000e-06	0.00389	0.209	0.133
sqr_000_03321	MnPt	2	-7.371	-7.547	-1.000e-06	0.00408	0.161	0.162

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_03322	AgYb	2	-2.393	-2.528	1.800e-06	0.00139	0.301	0.281
sqr_000_03324	RhTb	2	-6.692	-6.748	-3.600e-05	0.00638	0.113	0.065
sqr_000_03327	AuCo	2	-4.408	-4.684	-3.190e-05	0.00701	0.328	0.152
sqr_000_03337	YbZn	2	-1.524	-1.625	-1.790e-05	0.00126	0.26	0.111
sqr_000_03338	GdPd	2	-5.724	-5.751	-5.000e-06	0.00176	0.101	0.109
sqr_000_03342	BiGd	2	-4.764	-4.952	1.000e-07	0.001	0.428	0.189
sqr_000_03343	NiV	2	-7.399	-7.412	-1.000e-06	0.00608	0.054	0.054
sqr_000_03344	FeRu	2	-8.336	-8.556	-2.000e-06	0.00166	0.165	0.139
sqr_000_03348	IrRu	2	-8.789	-9.069	1.000e-06	0.00257	0.213	0.231
sqr_000_03349	TbZr	2	-6.243	-6.379	3.000e-06	0.00184	0.54	0.395
sqr_000_03351	Ir ₂ NdTa	4	-8.258	-8.857	-1.000e-06	0.00411	0.929	0.941
sqr_000_03352	Ru ₂	2	-7.888	-9.0	-3.000e-06	0.0044	0.237	0.376
sqr_000_03355	RhRu	2	-7.774	-8.168	-1.000e-06	0.00614	0.201	0.217
sqr_000_03356	CdNdTe ₂	4	-3.315	-3.921	0.000e+00	0.00453	0.772	1.087
sqr_000_03359	GdZr	2	-6.263	-6.394	-7.000e-06	0.00311	0.623	0.617
sqr_000_03365	GdRh	2	-6.648	-6.729	1.000e-06	0.00053	0.145	0.044
sqr_000_03367	NdZn	2	-3.096	-3.224	-1.000e-05	0.00441	0.237	0.122
sqr_000_03369	DyEu	2	-2.969	-2.994	-1.352e-02	0.00794	0.156	0.098
sqr_000_03375	PrYb	2	-2.983	-3.016	7.000e-07	0.00319	0.148	0.155
sqr_000_03376	DySn	2	-4.734	-4.812	-5.000e-07	0.00093	0.415	0.238
sqr_000_03380	AlRu	2	-6.266	-7.1	-2.000e-06	0.0003	0.248	0.166
sqr_000_03381	DyMg	2	-2.97	-3.098	-1.390e-05	0.00153	0.223	0.178
sqr_000_03383	AlNiRhYb	4	-4.891	-4.91	0.000e+00	0.00698	0.159	0.109
sqr_000_03385	AgGd	2	-3.907	-3.985	-5.300e-06	0.00623	0.167	0.108
sqr_000_03389	TbTe	2	-4.915	-5.043	-8.000e-06	0.0016	0.249	0.29
sqr_000_03390	CoRu	2	-7.346	-7.935	-3.000e-06	0.00396	0.214	0.167
sqr_000_03393	GaGdNbZn	4	-3.959	-4.785	-4.000e-06	0.00622	0.464	0.519
sqr_000_03395	SbYb	2	-3.294	-3.622	-1.900e-06	0.0004	0.57	0.382
sqr_000_03401	AlYb	2	-2.747	-2.793	-1.100e-06	0.00393	0.156	0.127
sqr_000_03404	DyTb	2	-4.279	-4.509	-1.870e-05	0.00328	0.44	0.366
sqr_000_03405	NdSc	2	-5.344	-5.424	-3.000e-06	0.00036	0.277	0.483
sqr_000_03407	NiSiZn	3	-3.956	-4.151	1.000e-06	0.0044	0.362	0.31
sqr_000_03414	FeIn	2	-4.783	-4.943	-3.800e-06	0.00379	0.262	0.165
sqr_000_03417	MgYb	2	-1.52	-1.529	-1.700e-06	0.002	0.153	0.101
sqr_000_03419	GdTe	2	-4.568	-5.09	-2.000e-06	0.00156	0.474	0.354
sqr_000_03421	GaGd	2	-3.874	-4.344	-4.000e-07	0.00015	0.454	0.315
sqr_000_03427	NdTl	2	-3.809	-3.864	-5.400e-06	0.00112	0.135	0.125
sqr_000_03432	MgTb	2	-3.035	-3.122	-8.000e-07	0.00035	0.502	0.368
sqr_000_03435	NdPt	2	-6.43	-6.442	-3.000e-06	0.00533	0.051	0.042
sqr_000_03436	GdTe	2	-4.991	-5.084	-1.000e-06	0.0015	0.242	0.235
sqr_000_03441	GaMgNpTb	4	-4.728	-5.012	-2.000e-06	0.00372	0.323	0.339
sqr_000_03446	BRu	2	-8.289	-8.292	-1.000e-06	0.00654	0.016	0.015
sqr_000_03447	AlDy	2	-4.227	-4.54	-1.000e-07	0.00251	0.367	0.151
sqr_000_03449	GdIr	2	-7.322	-7.486	-1.000e-06	0.00372	0.175	0.085
sqr_000_03452	FeV	2	-8.501	-8.704	-5.000e-06	0.00129	0.198	0.147
sqr_000_03453	MgTb	2	-3.088	-3.122	-3.900e-06	0.00194	0.135	0.091
sqr_000_03456	CdNd	2	-2.955	-3.058	-1.600e-06	0.00272	0.238	0.218
sqr_000_03460	AgNd	2	-3.855	-4.0	-1.300e-06	0.003	0.245	0.111
sqr_000_03461	GaGdMg ₂	4	-2.597	-2.792	0.000e+00	0.00443	0.383	0.251
sqr_000_03469	CdGd	2	-2.941	-2.99	-3.800e-06	0.00342	0.125	0.059
sqr_000_03470	AuGd	2	-4.734	-4.767	-5.900e-06	0.00162	0.105	0.083
sqr_000_03474	FePt	2	-6.929	-7.063	-3.900e-05	0.00741	0.19	0.208

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_03477	CoMn	2	-7.693	-7.948	-1.600e-05	0.00646	0.292	0.268
sqr_000_03480	NdSe	2	-5.166	-5.729	0.000e+00	0.00185	0.482	0.328
sqr_000_03482	NdTh	2	-5.946	-5.995	0.000e+00	0.00142	0.241	0.249
sqr_000_03485	DyHo	2	-4.326	-4.483	-1.770e-05	0.0009	0.261	0.533
sqr_000_03492	HfRu	2	-9.918	-10.353	1.000e-06	0.00148	0.312	0.168
sqr_000_03499	FeRu	2	-8.247	-8.549	0.000e+00	0.00303	0.299	0.167
sqr_000_03500	AgNd	2	-3.935	-3.997	-6.000e-07	0.00064	0.158	0.085
sqr_000_03501	AgDy	2	-3.539	-3.98	-1.200e-06	0.00209	0.432	0.186
sqr_000_03502	DyIn	2	-4.006	-4.026	0.000e+00	0.00064	0.091	0.067
sqr_000_03504	Ga ₃ Mn	4	-3.975	-4.188	1.000e-06	0.00878	0.231	0.194
sqr_000_03507	DySb	2	-4.411	-5.23	1.000e-06	0.00374	0.486	0.248
sqr_000_03509	GdSb	2	-5.13	-5.518	-5.000e-06	0.00048	1.432	0.523
sqr_000_03513	EuYb	2	-1.635	-1.66	-3.000e-07	0.00224	0.156	0.152
sqr_000_03515	DyMg	2	-3.012	-3.098	2.000e-07	0.00045	0.192	0.143
sqr_000_03516	GdMg	2	-3.113	-3.141	-9.500e-06	0.00026	0.121	0.104
sqr_000_03518	NiPRu	3	-6.614	-6.955	-1.000e-06	0.00555	0.443	0.492
sqr_000_03519	AuNd	2	-4.739	-4.751	-4.700e-06	0.0018	0.086	0.073
sqr_000_03521	FePd	2	-6.303	-6.351	1.000e-06	0.003	0.15	0.181
sqr_000_03522	RhTb	2	-6.691	-6.748	-3.000e-06	0.00161	0.113	0.069
sqr_000_03524	BiYb	2	-3.408	-3.41	1.200e-06	0.00268	0.029	0.023
sqr_000_03528	BrTb	2	-3.864	-3.878	4.500e-06	0.00116	0.078	0.04
sqr_000_03529	CuNdPt ₂	4	-5.427	-5.787	-1.200e-05	0.00543	0.752	2.601
sqr_000_03531	IrTb	2	-7.37	-7.512	-6.200e-05	0.00258	0.159	0.094
sqr_000_03534	CoNi	2	-5.906	-6.083	1.000e-06	0.00683	0.385	0.563
sqr_000_03559	NdZr	2	-6.339	-6.411	0.000e+00	0.00251	0.344	0.193
sqr_000_03563	MnPt	2	-7.421	-7.551	-9.000e-06	0.00771	0.182	0.201
sqr_000_03564	RuZr	2	-9.086	-9.499	-1.000e-06	0.00015	0.364	0.328
sqr_000_03566	AsDyGa	3	-4.568	-4.676	-1.000e-06	0.00297	0.302	0.225
sqr_000_03567	AsTb	2	-5.42	-6.144	-1.000e-06	0.00036	1.315	0.975
sqr_000_03569	DyNd	2	-3.999	-4.591	0.000e+00	0.00108	0.464	0.498
sqr_000_03573	GdSc	2	-5.329	-5.367	3.000e-06	0.00116	0.399	0.278
sqr_000_03575	DyPtSi	3	-5.782	-6.077	2.000e-06	0.00425	0.48	0.572
sqr_000_03580	TbZn	2	-3.174	-3.183	-1.800e-06	0.004	0.056	0.035
sqr_000_03583	SbYb	2	-3.203	-3.638	-1.320e-05	0.00444	0.812	0.7
sqr_000_03585	SeYb	2	-3.309	-4.573	-1.000e-07	0.00164	0.875	0.613
sqr_000_03588	GdTe	2	-4.684	-5.09	0.000e+00	0.00669	0.402	0.219
sqr_000_03594	Mg ₃ Tb	4	-1.719	-2.323	-2.100e-06	0.00407	0.557	0.322
sqr_000_03603	Gd ₂	2	-4.239	-4.551	-1.600e-06	0.00047	0.442	0.456
sqr_000_03604	FeGa	2	-5.49	-5.612	-3.000e-06	0.00777	0.146	0.098
sqr_000_03605	LiNd	2	-3.118	-3.166	8.000e-06	0.00301	0.206	0.108
sqr_000_03611	NiPdTbYb	4	-5.117	-5.278	-1.100e-05	0.0081	1.049	0.575
sqr_000_03612	CoNi	2	-6.057	-6.071	0.000e+00	0.00243	0.065	0.062
sqr_000_03613	TbZn	2	-3.179	-3.182	1.000e-07	0.00252	0.03	0.022
sqr_000_03614	MgYb	2	-1.512	-1.526	-3.330e-05	0.00401	0.139	0.101
sqr_000_03616	IrPt ₂ Yb	4	-6.042	-6.157	-4.000e-06	0.00509	0.142	0.124
sqr_000_03617	CdTbTi	3	-3.958	-4.236	-4.000e-06	0.00498	0.725	0.441
sqr_000_03620	InTb	2	-4.028	-4.051	3.400e-06	0.00081	0.096	0.077
sqr_000_03622	PtRu	2	-7.527	-7.593	-3.000e-06	0.00329	0.118	0.107
sqr_000_03626	CaIDyS	4	-4.61	-5.928	-2.000e-06	0.00686	0.855	2.312
sqr_000_03628	GdPtScTc	4	-6.27	-7.334	-2.000e-06	0.0052	0.574	0.652
sqr_000_03631	AgGdMgRu	4	-4.322	-4.49	-1.000e-06	0.00259	0.455	0.497
sqr_000_03632	DyHg	2	-2.499	-2.867	-1.600e-06	0.00147	0.386	0.248

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_03638	CdNd	2	-2.64	-3.061	7.600e-06	0.00143	0.479	0.248
sqr_000_03643	BeRu	2	-6.635	-6.664	-5.000e-06	0.00516	0.058	0.039
sqr_000_03645	PdYb	2	-3.926	-4.204	-8.000e-07	0.00092	0.359	0.261
sqr_000_03647	CdNd	2	-3.032	-3.048	1.000e-06	0.00273	0.085	0.049
sqr_000_03649	Cd ₂ SnTb	4	-2.8	-2.896	-1.000e-06	0.00298	0.2	0.161
sqr_000_03650	BaYb	2	-1.492	-1.658	-1.200e-06	0.00175	0.437	0.392
sqr_000_03651	AgYb	2	-2.452	-2.525	-1.830e-05	0.00203	0.218	0.168
sqr_000_03658	NdP	2	-5.932	-6.598	-2.000e-06	0.00303	1.187	1.171
sqr_000_03660	NiPt	2	-5.788	-5.862	-8.000e-05	0.00783	0.085	0.045
sqr_000_03663	MgRu	2	-4.966	-5.114	-6.000e-06	0.00096	0.181	0.099
sqr_000_03664	CdYb	2	-1.495	-1.519	-5.700e-06	0.00072	0.127	0.1
sqr_000_03672	AgGd	2	-3.98	-3.984	7.000e-07	0.00259	0.055	0.056
sqr_000_03681	GdSb	2	-4.373	-5.525	-4.000e-06	0.00267	1.474	0.917
sqr_000_03683	Co ₂	2	-6.812	-6.841	-3.000e-06	0.00544	0.054	0.026
sqr_000_03689	GdPt	2	-6.463	-6.51	0.000e+00	0.00179	0.148	0.115
sqr_000_03690	RhRu	2	-7.465	-8.093	0.000e+00	0.00534	0.282	0.266
sqr_000_03694	SeYb	2	-4.121	-4.262	-2.900e-06	0.0024	0.248	0.155
sqr_000_03701	NbNi	2	-7.711	-7.99	-6.000e-06	0.00531	0.231	0.222
sqr_000_03702	TlYb	2	-2.151	-2.357	-6.000e-07	0.0026	0.496	0.334
sqr_000_03706	GdP	2	-6.042	-6.597	-3.000e-06	0.00109	1.32	0.443
sqr_000_03709	RuTi	2	-8.974	-9.26	0.000e+00	0.00276	0.215	0.144
sqr_000_03710	GdTl	2	-3.337	-3.791	-7.900e-06	0.00157	0.484	0.279
sqr_000_03713	AuDy	2	-4.731	-4.758	-9.000e-07	0.00197	0.115	0.043
sqr_000_03715	SbTb	2	-4.551	-5.494	1.000e-06	0.00074	1.465	1.098
sqr_000_03717	MnPt	2	-7.493	-7.552	0.000e+00	0.00466	0.119	0.091
sqr_000_03720	AgGd	2	-3.972	-3.984	-5.000e-06	0.00137	0.06	0.046
sqr_000_03723	Yb ₂	2	-1.337	-1.448	-2.900e-06	0.00481	0.299	0.174
sqr_000_03724	GdSb	2	-5.047	-5.5	0.000e+00	0.00245	1.453	1.16
sqr_000_03727	DyTl	2	-3.719	-3.732	1.800e-06	0.00192	0.072	0.035
sqr_000_03729	ErGd	2	-4.297	-4.497	-4.900e-06	0.00231	0.454	0.591
sqr_000_03730	GdNd	2	-4.513	-4.643	-2.240e-05	0.00067	0.609	0.591
sqr_000_03734	AlCo	2	-5.88	-5.988	1.000e-06	0.0028	0.213	0.144
sqr_000_03746	CoNi	2	-6.05	-6.07	-1.700e-05	0.00239	0.084	0.132
sqr_000_03747	AgGaYbZn	4	-2.114	-2.369	5.000e-07	0.0088	1.006	0.855
sqr_000_03754	AgAl ₂ Gd	4	-3.35	-3.975	-1.000e-06	0.00158	0.399	0.343
sqr_000_03755	HgNd	2	-2.804	-2.917	-2.800e-05	0.0032	0.182	0.117
sqr_000_03756	TlYb	2	-2.33	-2.342	5.000e-07	0.00203	0.101	0.097
sqr_000_03759	TlYb	2	-2.235	-2.352	-2.500e-06	0.00171	0.28	0.199
sqr_000_03763	GdHg	2	-2.871	-2.875	-2.300e-06	0.00314	0.044	0.081
sqr_000_03770	BeMn	2	-6.268	-6.288	-8.000e-06	0.00088	0.055	0.034
sqr_000_03771	CoFe	2	-7.364	-7.457	-1.800e-05	0.00406	0.154	0.091
sqr_000_03772	DyNa	2	-2.393	-2.472	7.000e-07	0.00542	0.222	0.142
sqr_000_03778	NdNiPtTa	4	-6.639	-7.321	0.000e+00	0.00684	0.801	1.579
sqr_000_03781	AgNd	2	-3.968	-3.993	5.000e-07	0.00076	0.095	0.059
sqr_000_03786	NdTm	2	-4.443	-4.568	5.000e-07	0.00141	0.504	0.291
sqr_000_03787	SbYb	2	-3.282	-3.641	-4.400e-06	0.00429	0.614	0.606
sqr_000_03792	NdZr	2	-6.274	-6.344	8.000e-06	0.00155	0.2	0.184
sqr_000_03802	DyRh	2	-6.711	-6.767	1.000e-06	0.0034	0.11	0.077
sqr_000_03804	GeTb	2	-5.142	-5.238	-1.100e-05	0.00392	0.442	0.415
sqr_000_03806	AgDy	2	-3.532	-3.98	2.000e-07	0.0032	0.439	0.215
sqr_000_03808	NdSb	2	-5.033	-5.607	-1.000e-06	0.00176	1.424	1.1
sqr_000_03811	DyZn	2	-3.13	-3.172	-1.000e-07	0.00416	0.122	0.101

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_03814	GdPPt	3	-6.699	-6.724	-3.000e-06	0.00494	0.13	0.067
sqr_000_03817	HgYb	2	-1.13	-1.495	0.000e+00	0.00192	0.548	0.637
sqr_000_03819	SbYb	2	-3.449	-3.593	2.700e-06	0.0012	0.278	0.191
sqr_000_03821	DyIn	2	-3.911	-4.015	-2.500e-06	0.00302	0.174	0.082
sqr_000_03822	SbTb	2	-4.976	-5.495	0.000e+00	0.00426	1.28	0.917
sqr_000_03824	PdRu	2	-6.579	-6.941	3.000e-06	0.00308	0.447	0.645
sqr_000_03825	PTb	2	-5.937	-6.592	-6.000e-06	0.00262	1.276	0.909
sqr_000_03842	AlYb	2	-2.746	-2.793	1.000e-07	0.00141	0.158	0.103
sqr_000_03846	PdRh ₂ Yb	4	-5.644	-5.689	-2.000e-06	0.00498	0.109	0.104
sqr_000_03848	RuTa	2	-10.32	-10.79	-8.900e-05	0.00101	0.395	0.372
sqr_000_03856	MgYb	2	-1.513	-1.526	-1.560e-05	0.00079	0.127	0.083
sqr_000_03859	RuSc	2	-7.936	-8.251	-1.000e-06	0.00149	0.415	0.353
sqr_000_03860	RuZr	2	-9.315	-9.537	-1.000e-05	0.00145	0.158	0.173
sqr_000_03861	BeCo	2	-5.59	-5.698	-2.000e-06	0.00077	0.143	0.122
sqr_000_03862	AsVYb	3	-5.168	-5.282	-1.000e-06	0.00209	0.216	0.139
sqr_000_03866	RuTa	2	-10.564	-10.815	-1.000e-06	0.00265	0.151	0.198
sqr_000_03871	RuZr	2	-9.44	-9.523	-1.000e-06	0.00074	0.189	0.176
sqr_000_03872	CdDy	2	-2.929	-2.963	-1.280e-05	0.00181	0.158	0.093
sqr_000_03873	NdPd	2	-5.667	-5.696	1.000e-05	0.0014	0.093	0.074
sqr_000_03877	RhRu	2	-7.788	-8.162	-5.000e-06	0.00796	0.266	0.227
sqr_000_03881	SnYb	2	-2.937	-3.304	0.000e+00	0.00651	0.503	0.389
sqr_000_03885	STb	2	-5.945	-6.008	-2.300e-05	0.00614	0.136	0.122
sqr_000_03888	LiPtSbTb	4	-4.882	-4.963	-1.000e-05	0.00607	0.171	0.246
sqr_000_03890	CoFe	2	-7.331	-7.456	1.000e-06	0.00435	0.215	0.202
sqr_000_03898	NiRh	2	-6.196	-6.304	-1.000e-06	0.00327	0.393	0.182
sqr_000_03900	Ag ₂ Nd	3	-3.581	-3.656	-1.000e-05	0.00521	0.29	0.199
sqr_000_03903	GdZn	2	-3.164	-3.192	-1.090e-05	0.00103	0.136	0.112
sqr_000_03905	CdNd	2	-2.945	-3.043	0.000e+00	0.00211	0.179	0.113
sqr_000_03907	GaRu	2	-6.141	-6.344	-5.000e-06	0.00133	0.172	0.112
sqr_000_03908	CrNi	2	-6.686	-7.448	-2.700e-05	0.00516	0.34	0.308
sqr_000_03914	TbZn	2	-3.178	-3.182	-1.930e-05	0.00092	0.055	0.05
sqr_000_03915	BaYb	2	-1.338	-1.653	3.100e-06	0.00322	0.567	0.287
sqr_000_03918	NdPt	2	-6.403	-6.44	-9.000e-06	0.00205	0.195	0.126
sqr_000_03921	CdGd	2	-2.833	-3.003	-1.800e-06	0.00315	0.265	0.124
sqr_000_03922	RuTh	2	-8.436	-8.645	-2.700e-05	0.00113	0.187	0.084
sqr_000_03938	GdZn	2	-3.191	-3.192	2.000e-07	0.00158	0.019	0.02
sqr_000_03939	DyTi	2	-5.798	-5.887	0.000e+00	0.0022	0.47	0.241
sqr_000_03944	AsGd	2	-5.726	-6.153	-3.000e-06	0.00059	1.254	1.29
sqr_000_03945	Rh ₃ Yb	4	-6.113	-6.135	-1.200e-05	0.00365	0.068	0.069
sqr_000_03946	BiTb	2	-4.711	-4.91	-6.000e-06	0.0017	0.439	0.3
sqr_000_03948	CDyZn	3	-4.109	-4.944	0.000e+00	0.00346	1.035	1.825
sqr_000_03950	DyPtSnZn	4	-4.136	-4.507	0.000e+00	0.00496	0.338	0.298
sqr_000_03954	AlMnSc	3	-5.779	-6.445	-1.100e-05	0.00586	0.747	0.706
sqr_000_03956	TbTe	2	-5.017	-5.04	-3.000e-06	0.00607	0.091	0.054
sqr_000_03958	MnRh	2	-8.066	-8.093	3.000e-06	0.00077	0.059	0.041
sqr_000_03959	Dy ₂	2	-4.034	-4.465	-4.917e-04	0.0017	0.376	0.444
sqr_000_03961	AgGd	2	-3.971	-3.984	-1.900e-06	0.0033	0.082	0.069
sqr_000_03962	Ni ₂	2	-5.336	-5.411	-1.300e-05	0.00321	0.147	0.125
sqr_000_03964	NdZn	2	-3.212	-3.221	-6.800e-06	0.00489	0.057	0.047
sqr_000_03965	Rh ₃ Tb	4	-6.825	-7.049	-1.900e-05	0.00574	0.194	0.178
sqr_000_03967	DyPd	2	-5.758	-5.762	-1.000e-06	0.00275	0.032	0.018
sqr_000_03970	DyTe	2	-4.991	-4.993	-1.400e-06	0.00164	0.028	0.016

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_03971	HfOsRu	3	-9.844	-10.173	0.000e+00	0.0023	0.186	0.134
sqr_000_03972	Ni ₂	2	-5.275	-5.402	-1.000e-06	0.00307	0.312	1.557
sqr_000_03976	NiRe	2	-8.285	-8.867	-2.000e-06	0.00764	0.279	0.461
sqr_000_03982	DyTi ₃	4	-5.606	-6.705	-1.600e-05	0.00565	0.559	0.444
sqr_000_03983	CoZn	2	-3.953	-4.021	-2.100e-06	0.00116	0.109	0.088
sqr_000_03984	CdYb	2	-1.5	-1.517	2.300e-06	0.00442	0.096	0.066
sqr_000_03988	SbTb	2	-4.9	-5.493	0.000e+00	0.00307	1.402	1.144
sqr_000_03993	FeRu	2	-8.234	-8.55	-2.000e-05	0.00526	0.426	0.29
sqr_000_03996	CoGa	2	-5.176	-5.239	-3.000e-06	0.00237	0.114	0.117
sqr_000_03997	MgNd	2	-3.192	-3.215	-6.000e-07	0.00048	0.102	0.068
sqr_000_04004	AsNd	2	-5.446	-6.194	-4.000e-06	0.00608	1.294	1.267
sqr_000_04009	MoNiRu	3	-8.295	-8.486	-2.600e-05	0.00372	0.262	0.288
sqr_000_04010	MnNi	2	-6.919	-7.133	-4.800e-05	0.00885	0.32	0.268
sqr_000_04028	NdZn	2	-3.197	-3.223	7.000e-07	0.00163	0.133	0.142
sqr_000_04033	Cu ₂ RhTb	4	-5.112	-5.174	-2.400e-05	0.00616	0.347	0.305
sqr_000_04035	NaTb	2	-2.192	-2.493	2.700e-06	0.00972	0.419	0.301
sqr_000_04038	Fe ₂	2	-7.984	-8.077	-6.000e-06	0.00152	0.169	0.205
sqr_000_04046	MgTb	2	-3.101	-3.122	-2.400e-06	0.00058	0.104	0.054
sqr_000_04048	FeZn	2	-4.19	-4.326	-1.740e-05	0.00029	0.156	0.113
sqr_000_04052	Be ₃ Gd	4	-3.355	-3.744	-2.000e-06	0.00226	0.633	0.345
sqr_000_04053	GdHg	2	-2.393	-2.897	-6.800e-06	0.00186	0.49	0.176
sqr_000_04054	DyY	2	-5.315	-5.458	0.000e+00	0.00133	0.557	0.773
sqr_000_04058	FeZn	2	-4.237	-4.341	-1.500e-06	0.00527	0.205	0.206
sqr_000_04059	DyPt ₃	4	-6.709	-6.716	0.000e+00	0.0044	0.047	0.032
sqr_000_04060	AuTb	2	-4.709	-4.763	1.000e-07	0.0016	0.118	0.066
sqr_000_04062	TbTl	2	-3.676	-3.752	-2.600e-06	0.00263	0.247	0.175
sqr_000_04063	MnMo	2	-9.777	-9.797	1.000e-06	0.00935	0.049	0.033
sqr_000_04064	TeYb	2	-3.674	-3.963	-2.000e-07	0.00387	1.454	1.696
sqr_000_04065	RhRu	2	-7.72	-8.115	-1.000e-06	0.00618	0.4	0.438
sqr_000_04068	HgNd	2	-2.872	-2.92	-2.000e-06	0.00066	0.169	0.106
sqr_000_04078	GdPt ₂	3	-6.328	-6.432	-2.000e-06	0.0042	0.327	0.361
sqr_000_04079	PrRu	2	-6.814	-6.95	-1.000e-06	0.00218	0.156	0.135
sqr_000_04082	GdReSi	3	-7.09	-7.709	-1.000e-06	0.00427	0.554	0.528
sqr_000_04084	NdS	2	-5.992	-6.152	-1.000e-06	0.00236	0.307	0.245
sqr_000_04085	CeMgTb	3	-3.836	-3.961	1.700e-05	0.0051	0.41	0.303
sqr_000_04090	CuNi	2	-4.474	-4.517	-7.200e-06	0.0029	0.119	0.102
sqr_000_04095	IrNi	2	-6.909	-7.117	-1.000e-06	0.00675	0.187	0.124
sqr_000_04100	HgYb	2	-1.434	-1.476	-2.600e-06	0.00183	0.152	0.094
sqr_000_04101	GdS	2	-5.862	-6.044	-3.000e-06	0.0023	0.227	0.123
sqr_000_04107	NdU	2	-6.801	-7.262	-1.000e-06	0.00557	1.018	0.698
sqr_000_04109	FeZn	2	-4.193	-4.347	1.500e-06	0.00256	0.147	0.093
sqr_000_04112	SrYb	2	-1.121	-1.513	-5.000e-07	0.00162	0.579	0.357
sqr_000_04118	HgYb	2	-1.427	-1.477	4.000e-07	0.0017	0.169	0.15
sqr_000_04120	DySm	2	-4.453	-4.577	1.900e-06	0.00162	0.609	0.408
sqr_000_04122	AsTb	2	-5.628	-6.135	-1.000e-06	0.00061	1.308	1.298
sqr_000_04129	GdZn	2	-3.056	-3.191	-3.600e-06	0.00311	0.235	0.104
sqr_000_04130	GaTb	2	-4.319	-4.32	1.000e-07	0.00911	0.017	0.015
sqr_000_04132	PdRu	2	-6.655	-6.949	0.000e+00	0.00884	0.561	1.801
sqr_000_04135	CuDy	2	-4.349	-4.397	-4.010e-05	0.00442	0.122	0.071
sqr_000_04139	GdTl	2	-3.727	-3.778	-3.800e-06	0.00217	0.124	0.076
sqr_000_04140	FeRh	2	-7.569	-7.616	-4.000e-06	0.00281	0.092	0.123
sqr_000_04143	SbYb	2	-3.584	-3.593	1.000e-06	0.00405	0.132	0.125

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_04153	DyU	2	-6.812	-7.344	-2.000e-06	0.0046	0.941	1.105
sqr_000_04161	Ni ₂	2	-5.318	-5.408	-2.000e-06	0.00455	0.14	0.1
sqr_000_04162	DySe	2	-5.497	-5.514	-3.000e-06	0.00069	0.112	0.096
sqr_000_04163	FeGa	2	-5.401	-5.598	-6.000e-06	0.00449	0.377	0.4
sqr_000_04165	CoHf	2	-8.858	-8.86	5.000e-06	0.00283	0.04	0.028
sqr_000_04168	Ru ₂	2	-8.425	-9.06	-9.000e-06	0.00404	0.237	0.285
sqr_000_04170	NiTi	2	-6.734	-6.975	-6.000e-06	0.00337	0.441	0.28
sqr_000_04173	SeTb	2	-5.556	-5.559	-2.000e-06	0.00241	0.033	0.026
sqr_000_04174	NdSe	2	-5.402	-5.733	-2.000e-06	0.0045	0.343	0.237
sqr_000_04175	AlNi	2	-5.143	-5.275	0.000e+00	0.00393	0.154	0.068
sqr_000_04178	GdGeTm	3	-4.508	-4.918	1.000e-06	0.00583	0.273	0.685
sqr_000_04181	AsCuGdLi	4	-4.141	-4.312	-1.000e-06	0.00346	0.878	1.038
sqr_000_04184	Be ₂ CoMn	4	-3.92	-5.911	0.000e+00	0.00814	0.523	0.548
sqr_000_04185	RuTi	2	-8.667	-9.255	-2.000e-06	0.00156	0.529	0.502
sqr_000_04192	DyNa	2	-2.469	-2.477	9.000e-07	0.00264	0.075	0.046
sqr_000_04206	BeDyFe	3	-5.402	-5.442	-2.900e-05	0.00415	0.164	0.168
sqr_000_04208	MgTb	2	-3.102	-3.122	-3.000e-06	0.0013	0.099	0.095
sqr_000_04210	LiNi	2	-3.499	-3.547	-2.000e-07	0.00278	0.139	0.136
sqr_000_04215	DySc	2	-5.258	-5.299	1.000e-06	0.00233	0.125	0.096
sqr_000_04216	GaPaTbW	4	-7.008	-7.252	0.000e+00	0.00358	0.491	0.369
sqr_000_04218	BiNiTb	3	-4.839	-5.132	-2.780e-04	0.00598	0.224	0.17
sqr_000_04225	GdY	2	-5.397	-5.496	-9.000e-06	0.00407	0.442	0.339
sqr_000_04228	AgYb	2	-2.455	-2.525	-1.820e-05	0.00322	0.21	0.163
sqr_000_04232	HfNi	2	-7.606	-8.116	-4.200e-05	0.00834	0.493	0.377
sqr_000_04236	DyHg	2	-2.537	-2.866	1.500e-06	0.00044	0.361	0.212
sqr_000_04237	AlU ₂ Yb	4	-5.906	-6.619	-2.000e-06	0.00212	0.547	0.381
sqr_000_04240	Be ₃ Ni	4	-4.024	-4.452	0.000e+00	0.00604	0.331	0.173
sqr_000_04241	NiPt	2	-5.763	-5.863	-1.400e-05	0.00191	0.304	0.212
sqr_000_04244	CoLi	2	-4.026	-4.125	1.640e-05	0.00259	0.27	0.14
sqr_000_04246	NiTc	2	-7.399	-7.872	-3.000e-06	0.00244	0.327	0.359
sqr_000_04247	NiZn	2	-3.48	-3.539	-3.300e-06	0.00538	0.277	0.251
sqr_000_04249	PtTb	2	-6.505	-6.521	0.000e+00	0.00292	0.074	0.064
sqr_000_04256	TbU	2	-6.752	-7.3	-1.000e-06	0.00501	1.013	0.684
sqr_000_04259	GdRh	2	-6.381	-6.728	-1.360e-04	0.00052	0.295	0.212
sqr_000_04260	TbTl	2	-3.724	-3.763	1.000e-07	0.00164	0.128	0.078
sqr_000_04266	DyMg	2	-3.087	-3.103	6.000e-07	0.001	0.091	0.066
sqr_000_04267	NdYb	2	-2.972	-2.995	-2.000e-07	0.00079	0.116	0.085
sqr_000_04269	HNi	2	-4.021	-4.448	-1.520e-05	0.00134	0.682	0.638
sqr_000_04270	AgDy	2	-3.771	-3.975	-3.020e-05	0.00097	0.282	0.18
sqr_000_04273	GdRu	2	-6.083	-6.989	-4.000e-06	0.0029	0.515	0.385
sqr_000_04282	Ga ₂ Yb	3	-2.792	-2.979	2.870e-05	0.00425	0.345	0.228
sqr_000_04286	HgYb	2	-1.434	-1.476	3.000e-07	0.00266	0.151	0.151
sqr_000_04288	Ni ₃ Si	4	-5.489	-5.913	-6.000e-06	0.00568	0.24	0.157
sqr_000_04291	TbTe	2	-5.024	-5.04	0.000e+00	0.00108	0.075	0.051
sqr_000_04292	CoMn	2	-7.809	-7.959	-1.000e-06	0.00167	0.119	0.077
sqr_000_04298	Be ₃ Ru	4	-4.487	-5.386	-1.000e-06	0.004	0.541	1.154
sqr_000_04299	GdMg	2	-3.124	-3.14	-8.900e-06	0.00101	0.102	0.078
sqr_000_04300	LuRu	2	-6.753	-7.237	-1.000e-06	0.00043	0.371	0.234
sqr_000_04313	CaDy	2	-2.886	-3.039	-3.100e-06	0.00014	0.288	0.196
sqr_000_04322	SnYb	2	-3.236	-3.341	-1.800e-06	0.00405	0.521	0.31
sqr_000_04325	DyIr	2	-7.463	-7.533	-1.000e-06	0.00207	0.12	0.075
sqr_000_04326	AgDy	2	-3.966	-3.972	-1.200e-06	0.00382	0.044	0.032

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_04329	GaNi	2	-4.434	-4.549	-6.000e-07	0.00199	0.484	0.328
sqr_000_04332	Ir ₃ Tb	4	-7.734	-8.154	0.000e+00	0.00256	0.228	0.151
sqr_000_04334	AuTb	2	-4.761	-4.763	-1.330e-05	0.00511	0.026	0.021
sqr_000_04337	NiRu	2	-7.062	-7.205	0.000e+00	0.00695	0.194	0.123
sqr_000_04339	CoPt	2	-6.17	-6.486	-4.000e-06	0.00294	0.25	0.187
sqr_000_04341	MnNi	2	-6.816	-7.129	-1.795e-02	0.00276	0.314	0.369
sqr_000_04343	MgTb	2	-3.037	-3.119	-1.500e-06	0.00013	0.176	0.095
sqr_000_04344	TeYb	2	-3.657	-3.966	1.000e-07	0.00077	1.329	1.087
sqr_000_04345	GdYb	2	-2.804	-2.873	-2.000e-07	0.00023	0.195	0.106
sqr_000_04347	NiZn	2	-3.351	-3.535	-7.500e-06	0.00361	0.168	0.081
sqr_000_04350	GaRu	2	-6.24	-6.33	-5.700e-05	0.00736	0.2	0.175
sqr_000_04371	MnNb	2	-8.937	-9.712	-3.300e-05	0.0019	0.542	0.419
sqr_000_04372	CoRu	2	-7.796	-7.947	-3.000e-06	0.00846	0.162	0.134
sqr_000_04375	DyYb	2	-2.757	-2.834	-6.500e-06	0.00089	0.255	0.25
sqr_000_04377	GdMg	2	-3.112	-3.141	-2.000e-07	0.0034	0.118	0.071
sqr_000_04381	RuY	2	-7.27	-7.996	-3.000e-05	0.00536	0.459	0.41
sqr_000_04390	CdNd	2	-3.042	-3.054	-4.400e-06	0.00245	0.071	0.032
sqr_000_04397	CdTb	2	-2.728	-2.988	-4.100e-06	0.0037	0.386	0.259
sqr_000_04407	GdMgUZn	4	-3.794	-4.188	0.000e+00	0.00198	0.403	0.477
sqr_000_04408	FeRu	2	-8.105	-8.547	-1.000e-06	0.00268	0.458	0.314
sqr_000_04411	AgDySn ₂	4	-3.793	-4.164	0.000e+00	0.00652	0.409	0.48
sqr_000_04412	Cd ₂ Nd	3	-2.206	-2.411	-3.500e-06	0.00628	0.683	0.565
sqr_000_04413	CoTi	2	-7.51	-7.794	0.000e+00	0.00183	0.243	0.149
sqr_000_04418	DyHg	2	-2.85	-2.85	-2.480e-05	0.00043	0.016	0.02
sqr_000_04419	CoPt	2	-6.258	-6.487	-6.800e-05	0.00444	0.247	0.179
sqr_000_04423	FeRu	2	-8.173	-8.548	-1.000e-06	0.00329	0.174	0.255
sqr_000_04430	NdSb	2	-5.299	-5.598	-3.000e-06	0.00285	1.382	0.798
sqr_000_04431	FeZn	2	-4.282	-4.319	-3.000e-07	0.00184	0.202	0.238
sqr_000_04437	DyTh	2	-5.826	-5.952	3.000e-06	0.00103	0.601	0.464
sqr_000_04440	DyZn	2	-3.169	-3.171	-5.600e-06	0.00128	0.025	0.019
sqr_000_04443	AuYb	2	-3.152	-3.321	-3.800e-06	0.00176	0.295	0.182
sqr_000_04446	DyZr ₂	3	-6.72	-7.057	1.000e-06	0.00376	0.467	0.291
sqr_000_04448	DySe	2	-5.506	-5.514	-2.000e-06	0.00041	0.094	0.084
sqr_000_04454	NiRu	2	-6.963	-7.211	-2.000e-06	0.00288	0.442	0.391
sqr_000_04455	TbZn	2	-3.108	-3.18	-8.300e-06	0.00063	0.165	0.101
sqr_000_04456	NdTl	2	-3.781	-3.864	-7.400e-06	0.00103	0.161	0.107
sqr_000_04458	HfRu	2	-10.303	-10.379	-2.500e-05	0.00418	0.099	0.069
sqr_000_04460	MgNd	2	-3.137	-3.22	3.800e-06	0.00179	0.188	0.087
sqr_000_04462	CdNd	2	-3.016	-3.056	1.000e-06	0.00325	0.129	0.051
sqr_000_04464	AgNd	2	-3.961	-3.993	4.000e-07	0.00164	0.113	0.059
sqr_000_04475	HgTb	2	-2.765	-2.861	-1.390e-05	0.00128	0.162	0.1
sqr_000_04482	IrRu	2	-8.587	-9.059	-2.000e-06	0.00331	0.215	0.277
sqr_000_04483	InYb	2	-2.496	-2.527	-1.400e-06	0.00266	0.165	0.19
sqr_000_04485	RuV	2	-9.274	-9.344	-1.000e-06	0.00196	0.084	0.046
sqr_000_04486	GdS	2	-5.893	-6.044	0.000e+00	0.00446	0.202	0.154
sqr_000_04490	BeFe	2	-5.811	-6.033	-5.300e-04	0.00255	0.194	0.149
sqr_000_04497	MnPd	2	-6.514	-6.813	-6.000e-06	0.00295	0.363	0.461
sqr_000_04498	DyU	2	-6.819	-7.306	0.000e+00	0.00362	0.982	1.185
sqr_000_04499	NdPd	2	-5.7	-5.703	1.000e-06	0.00195	0.045	0.047
sqr_000_04501	Co ₂	2	-6.662	-6.841	-5.000e-06	0.00983	0.197	0.192
sqr_000_04502	EuNd	2	-2.933	-3.197	1.000e-07	0.00106	0.466	0.514
sqr_000_04503	SnYb	2	-3.263	-3.341	6.000e-07	0.00653	0.495	0.354

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_04505	HgYb	2	-1.413	-1.479	-5.100e-06	0.00109	0.2	0.121
sqr_000_04506	AgYb	2	-2.447	-2.525	-1.700e-06	0.00163	0.225	0.175
sqr_000_04508	In ₂ IrTb	4	-4.294	-4.929	0.000e+00	0.00329	0.383	0.431
sqr_000_04509	GdNi	2	-5.287	-5.39	-1.400e-05	0.00544	0.195	0.188
sqr_000_04510	TlYb	2	-2.338	-2.341	-3.000e-07	0.00077	0.047	0.038
sqr_000_04511	RuZr	2	-8.975	-9.499	1.000e-06	0.00145	0.255	0.154
sqr_000_04512	DyTh	2	-5.182	-5.928	1.700e-05	0.00267	0.505	0.519
sqr_000_04513	TbTe	2	-4.48	-5.046	1.000e-06	0.00386	0.493	0.348
sqr_000_04514	HfRu	2	-9.388	-10.283	-1.600e-05	0.00344	0.581	0.599
sqr_000_04518	BrGd	2	-3.878	-3.93	-8.000e-07	0.00064	0.163	0.057
sqr_000_04519	AuMn	2	-5.308	-5.54	-2.300e-05	0.00173	0.349	0.217
sqr_000_04520	CoNi	2	-6.023	-6.072	-1.000e-06	0.00449	0.169	0.146
sqr_000_04522	GdRh	2	-6.509	-6.723	-5.000e-06	0.00133	0.232	0.124
sqr_000_04524	NpRu	2	-9.713	-10.795	-1.000e-06	0.00727	0.678	0.622
sqr_000_04525	DySn	2	-4.653	-4.811	-4.380e-05	0.00655	0.314	0.429
sqr_000_04529	CFeLu	3	-7.375	-7.52	-2.000e-06	0.00547	0.156	0.057
sqr_000_04532	GdHg	2	-2.829	-2.872	-4.900e-06	0.00137	0.115	0.038
sqr_000_04537	MnRu	2	-8.717	-8.983	-1.000e-06	0.00337	0.432	0.306
sqr_000_04538	DyZn	2	-2.985	-3.172	-6.000e-07	0.00147	0.279	0.252
sqr_000_04541	CoPSnYb	4	-4.47	-4.953	-1.000e-06	0.00538	0.739	0.781
sqr_000_04546	GdIn	2	-4.035	-4.075	-1.900e-05	0.00184	0.125	0.055
sqr_000_04548	AgNd	2	-3.98	-3.994	-2.200e-05	0.00312	0.074	0.03
sqr_000_04550	NdSe	2	-5.203	-5.733	-1.000e-06	0.00187	0.461	0.319
sqr_000_04556	MnNb	2	-9.661	-9.73	-6.900e-05	0.00974	0.106	0.081
sqr_000_04558	GdTe	2	-5.079	-5.086	1.000e-06	0.0054	0.044	0.036
sqr_000_04560	HgTb	2	-2.701	-2.874	3.100e-06	0.00164	0.254	0.097
sqr_000_04564	MgNi	2	-3.586	-3.646	1.100e-06	0.00278	0.158	0.126
sqr_000_04566	BeRu	2	-6.351	-6.681	1.000e-06	0.00348	0.224	0.089
sqr_000_04581	HoMn	2	-6.126	-6.213	-3.000e-06	0.0028	0.166	0.117
sqr_000_04584	AlDyMgU	4	-4.431	-4.932	0.000e+00	0.00283	0.457	1.269
sqr_000_04587	MnZn	2	-4.657	-4.743	4.300e-06	0.00357	0.271	0.264
sqr_000_04588	CdCo	2	-2.795	-3.384	4.000e-07	0.00388	0.62	0.583
sqr_000_04590	Co ₃ Gd	4	-6.111	-6.135	-4.700e-05	0.00806	0.1	0.139
sqr_000_04598	AgDy	2	-3.953	-3.971	-1.400e-06	0.00622	0.071	0.052
sqr_000_04599	GdTe	2	-5.05	-5.086	0.000e+00	0.00247	0.174	0.11
sqr_000_04600	CdIrRuTb	4	-4.84	-5.938	-1.000e-06	0.00844	0.489	0.53
sqr_000_04604	GdLi	2	-3.079	-3.096	-2.800e-06	0.00156	0.106	0.056
sqr_000_04605	BiNd	2	-5.07	-5.084	-1.600e-05	0.00123	0.386	0.252
sqr_000_04608	AuNd	2	-4.699	-4.753	-1.300e-05	0.00233	0.126	0.108
sqr_000_04612	AlRu	2	-6.768	-7.119	-7.000e-06	0.00182	0.375	0.228
sqr_000_04613	TbTl	2	-3.16	-3.772	-1.079e-03	0.00639	0.577	0.383
sqr_000_04614	RhRu	2	-7.746	-8.15	0.000e+00	0.00231	0.268	0.292
sqr_000_04615	NiPt	2	-5.615	-5.857	-1.000e-06	0.00705	0.245	0.213
sqr_000_04616	GdZn	2	-3.182	-3.192	-3.000e-07	0.00103	0.083	0.091
sqr_000_04617	DyZr	2	-6.168	-6.359	2.300e-05	0.00191	0.488	0.343
sqr_000_04619	AgYb	2	-2.451	-2.525	2.800e-06	0.0008	0.222	0.128
sqr_000_04621	DyLi	2	-3.017	-3.065	-5.300e-06	0.00305	0.165	0.115
sqr_000_04626	HfNi	2	-7.815	-8.125	0.000e+00	0.00275	0.223	0.17
sqr_000_04628	TbYb	2	-2.783	-2.849	9.000e-07	0.00125	0.186	0.122
sqr_000_04629	GdRu	2	-6.934	-7.145	-7.000e-06	0.0004	0.236	0.194
sqr_000_04630	Ru ₂	2	-8.405	-9.041	-6.000e-06	0.00393	0.412	0.354
sqr_000_04632	BeNi	2	-5.077	-5.083	-5.000e-06	0.00671	0.049	0.036

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_04641	PtRu	2	-7.544	-7.587	0.000e+00	0.00542	0.071	0.061
sqr_000_04644	InNdTm ₂	4	-4.135	-4.311	1.000e-05	0.00078	0.382	0.385
sqr_000_04652	DyPt	2	-6.509	-6.531	0.000e+00	0.0022	0.067	0.026
sqr_000_04654	GdPd	2	-5.736	-5.75	-2.000e-06	0.00122	0.058	0.035
sqr_000_04659	DySb	2	-4.97	-5.446	0.000e+00	0.00143	1.389	1.37
sqr_000_04661	CNiRuZn	4	-5.81	-6.12	0.000e+00	0.0079	0.33	0.593
sqr_000_04664	AlYb	2	-2.749	-2.793	-1.600e-06	0.0015	0.153	0.112
sqr_000_04665	CoNi	2	-5.924	-6.065	-5.000e-06	0.00411	0.364	0.388
sqr_000_04671	MgNdPdRh	4	-4.758	-5.269	0.000e+00	0.00194	0.565	0.607
sqr_000_04673	NiSc	2	-6.177	-6.366	-1.000e-05	0.00567	0.306	0.252
sqr_000_04674	CoRu	2	-7.585	-7.95	-2.700e-05	0.00615	0.492	0.39
sqr_000_04675	AgGd	2	-3.962	-3.983	-8.000e-07	0.00077	0.092	0.075
sqr_000_04677	CoCr	2	-7.726	-8.225	-2.600e-05	0.00808	0.204	0.299
sqr_000_04683	InTb	2	-4.024	-4.043	1.300e-06	0.0011	0.075	0.051
sqr_000_04684	CoTi	2	-7.322	-7.786	-6.000e-05	0.00682	0.683	0.613
sqr_000_04686	RuTi	2	-9.273	-9.278	0.000e+00	0.00085	0.031	0.019
sqr_000_04692	AlGd	2	-4.171	-4.565	-7.000e-07	0.00267	0.417	0.26
sqr_000_04699	RuTb	2	-7.153	-7.154	1.000e-06	0.00158	0.024	0.019
sqr_000_04703	NdS	2	-6.074	-6.153	-4.000e-06	0.00195	0.282	0.212
sqr_000_04713	TbTl	2	-3.615	-3.751	-5.000e-07	0.00191	0.218	0.131
sqr_000_04714	NdYb	2	-2.838	-2.993	2.000e-07	0.00033	0.293	0.19
sqr_000_04715	RuZn	2	-4.988	-4.994	-7.100e-06	0.00098	0.03	0.017
sqr_000_04716	NiTm	2	-4.818	-5.421	-6.500e-05	0.00444	0.313	0.166
sqr_000_04719	NaYb	2	-1.142	-1.29	1.000e-06	0.00388	0.412	0.311
sqr_000_04723	DyYb	2	-2.744	-2.825	6.000e-07	0.00349	0.208	0.118
sqr_000_04728	CuTb	2	-4.333	-4.396	-1.300e-05	0.00859	0.189	0.125
sqr_000_04730	NdYb	2	-2.86	-2.994	-2.292e-04	0.00834	0.284	0.103
sqr_000_04731	CoNd	2	-5.577	-5.785	0.000e+00	0.00358	0.285	0.159
sqr_000_04734	GdRh	2	-6.323	-6.73	-9.000e-06	0.00198	0.323	0.206
sqr_000_04735	NdTl	2	-3.477	-3.877	-9.520e-05	0.00212	0.454	0.348
sqr_000_04738	MgYb	2	-1.52	-1.529	-4.000e-07	0.00133	0.156	0.137
sqr_000_04740	NdPdZn	3	-4.115	-4.207	-1.000e-05	0.00278	0.25	0.395
sqr_000_04744	BeMn	2	-6.198	-6.322	-1.000e-06	0.00181	0.145	0.11
sqr_000_04748	AgTb	2	-3.788	-3.982	-7.900e-06	0.00477	0.271	0.225
sqr_000_04749	DySb	2	-5.074	-5.457	1.000e-06	0.00051	1.403	1.4
sqr_000_04751	NdY	2	-5.433	-5.551	-4.400e-05	0.00054	0.56	0.371
sqr_000_04757	NiZn	2	-3.501	-3.541	1.110e-05	0.00652	0.233	0.174
sqr_000_04761	GdS	2	-5.911	-6.044	-7.000e-06	0.00204	0.191	0.145
sqr_000_04774	NiSc	2	-6.259	-6.356	-6.000e-06	0.00089	0.142	0.107
sqr_000_04777	CoMnSi	3	-7.241	-7.358	-4.500e-05	0.00208	0.161	0.213
sqr_000_04781	AgTb	2	-3.958	-3.978	-6.000e-07	0.00077	0.078	0.054
sqr_000_04783	FeRu	2	-8.136	-8.554	0.000e+00	0.00548	0.478	1.567
sqr_000_04790	MgNd	2	-3.213	-3.216	1.400e-06	0.00196	0.033	0.029
sqr_000_04791	DyEr	2	-4.188	-4.45	-1.600e-06	0.00404	0.447	0.773
sqr_000_04796	CuNd	2	-4.363	-4.369	-2.900e-06	0.0096	0.059	0.022
sqr_000_04799	SeTb	2	-4.695	-5.558	-4.000e-06	0.002	0.607	0.274
sqr_000_04801	GdGePd	3	-5.633	-5.732	-6.000e-06	0.00899	0.39	0.304
sqr_000_04802	InNd	2	-4.416	-3.938	-3.533e-04	0.00902	0.319	0.217
sqr_000_04803	GdZn	2	-3.18	-3.193	-6.600e-06	0.00191	0.087	0.065
sqr_000_04804	MgNd	2	-3.143	-3.217	1.100e-06	0.00187	0.216	0.167
sqr_000_04808	CoTi	2	-7.396	-7.787	-4.000e-06	0.00372	0.591	0.391
sqr_000_04813	MnRu	2	-8.757	-8.982	-5.000e-06	0.00638	0.266	0.27

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_04816	SrYb	2	-1.192	-1.514	5.000e-07	0.00036	0.514	0.324
sqr_000_04832	NdTl	2	-3.347	-3.878	5.600e-06	0.00447	0.544	0.321
sqr_000_04834	PdTb	2	-5.748	-5.756	1.000e-06	0.00254	0.064	0.05
sqr_000_04835	GdNi	2	-5.26	-5.389	2.000e-06	0.00228	0.295	0.194
sqr_000_04839	Co ₂ GaNd	4	-5.191	-5.391	-1.000e-06	0.00715	0.403	0.382
sqr_000_04844	AuDyFeZr	4	-6.085	-6.366	-4.000e-06	0.00815	0.69	2.542
sqr_000_04845	CoZn	2	-4.011	-4.016	-5.130e-05	0.00339	0.067	0.072
sqr_000_04846	GdSiTh	3	-5.259	-6.049	-1.000e-06	0.00244	0.518	0.77
sqr_000_04850	AlNi	2	-5.06	-5.266	-1.000e-06	0.00034	0.16	0.078
sqr_000_04854	AsNd	2	-5.769	-6.17	-1.000e-06	0.0038	1.268	1.144
sqr_000_04860	MgTb	2	-3.06	-3.119	0.000e+00	8e-05	0.157	0.058
sqr_000_04862	CoGdHfRh	4	-7.075	-7.637	-2.300e-05	0.00968	0.653	0.593
sqr_000_04868	Ga ₂ Yb	3	-2.932	-2.982	3.000e-07	0.00642	0.293	0.226
sqr_000_04869	GdRu	2	-7.042	-7.134	-1.000e-06	0.00145	0.137	0.073
sqr_000_04870	GdSm	2	-4.446	-4.607	5.000e-07	0.00292	0.587	0.427
sqr_000_04877	Ge ₂ Nd	3	-4.984	-5.163	-3.000e-06	0.0035	0.21	0.176
sqr_000_04879	CdDy	2	-2.948	-2.965	-1.200e-06	0.0034	0.068	0.04
sqr_000_04880	HgYb	2	-1.437	-1.475	-1.160e-05	0.0004	0.157	0.112
sqr_000_04883	Mg ₃ Yb	4	-1.22	-1.496	-4.800e-06	0.00378	0.451	0.297
sqr_000_04885	BeCo	2	-5.627	-5.696	0.000e+00	0.00227	0.101	0.097
sqr_000_04887	BeRu	2	-6.609	-6.668	-2.800e-05	0.00328	0.131	0.092
sqr_000_04890	DyNd	2	-4.534	-4.608	-4.360e-05	0.00637	0.2	0.292
sqr_000_04897	DyNd	2	-4.31	-4.604	-5.300e-06	0.00294	0.399	0.677
sqr_000_04899	AuYb	2	-3.17	-3.32	2.000e-07	0.00077	0.277	0.165
sqr_000_04917	MnRh	2	-7.737	-8.084	1.000e-06	0.00437	0.407	0.465
sqr_000_04923	HfRu	2	-10.181	-10.364	-3.000e-06	0.00367	0.148	0.074
sqr_000_04925	MgRu	2	-5.061	-5.119	-1.000e-06	0.00218	0.112	0.074
sqr_000_04926	FeRu	2	-8.527	-8.561	-7.000e-06	0.00052	0.092	0.068
sqr_000_04928	BeNi	2	-5.071	-5.081	-5.400e-05	0.00444	0.056	0.038
sqr_000_04930	AgDy	2	-3.938	-3.971	-6.000e-07	0.00137	0.112	0.038
sqr_000_04947	GdTe	2	-5.007	-5.086	0.000e+00	0.00425	0.186	0.139
sqr_000_04948	GdIr	2	-7.183	-7.474	-1.000e-06	0.00163	0.239	0.182
sqr_000_04950	NdPt	2	-6.422	-6.44	-8.000e-06	0.00436	0.137	0.077
sqr_000_04952	IrMn	2	-8.688	-9.028	-1.000e-06	0.00225	0.22	0.242
sqr_000_04957	Sc ₂ SiTb	4	-5.221	-5.901	0.000e+00	0.00764	0.474	0.41
sqr_000_04960	DyMg	2	-3.045	-3.101	0.000e+00	0.00079	0.306	0.385
sqr_000_04963	BeRu	2	-6.666	-6.671	-5.000e-06	0.00132	0.037	0.028
sqr_000_04964	DyIn	2	-3.938	-4.018	-8.900e-06	0.00342	0.21	0.164
sqr_000_04965	EuYb	2	-1.426	-1.653	-1.000e-07	0.00175	0.446	0.327
sqr_000_04970	MgNdTbTh	4	-4.269	-4.51	2.000e-06	0.00158	0.362	0.264
sqr_000_04971	BeNi	2	-5.017	-5.083	-1.100e-05	0.0046	0.101	0.06
sqr_000_04985	CuGdPr	3	-4.093	-4.308	0.000e+00	0.00413	0.557	0.652
sqr_000_04987	CdDy	2	-2.944	-2.966	-7.000e-06	0.0017	0.209	0.206
sqr_000_04990	FeV	2	-8.567	-8.711	-2.000e-06	0.0025	0.329	0.283
sqr_000_04992	DyHg ₂ Mg	4	-1.627	-1.997	-7.000e-07	0.00272	0.864	0.635
sqr_000_04994	SYb	2	-4.359	-5.052	0.000e+00	0.00458	1.192	1.116
sqr_000_04995	AuNdPdU	4	-5.894	-6.229	-2.000e-06	0.00525	1.189	0.643
sqr_000_04996	GdRh	2	-6.602	-6.731	-1.400e-05	0.00237	0.177	0.121
sqr_000_04997	CuGd	2	-4.16	-4.397	1.000e-07	0.00082	0.299	0.151
sqr_000_04998	TbTm	2	-4.185	-4.459	-3.700e-06	0.00173	0.496	0.278
sqr_000_05004	HMnOs	3	-3.798	-7.548	-5.000e-06	0.00459	0.494	0.571
sqr_000_05007	TmYb	2	-2.727	-2.771	-2.722e-04	0.00217	0.152	0.086

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_05009	YbZn	2	-1.531	-1.625	-2.100e-06	0.00048	0.253	0.176
sqr_000_05011	MgNdSn ₂	4	-2.313	-3.881	1.000e-06	0.00339	0.626	0.528
sqr_000_05012	SnTb	2	-4.616	-4.845	2.500e-06	0.00434	0.492	0.39
sqr_000_05013	HgNd	2	-2.882	-2.92	-3.000e-07	0.00164	0.175	0.119
sqr_000_05014	BaYb	2	-1.256	-1.652	-7.600e-06	0.00265	0.638	0.351
sqr_000_05015	AuDy	2	-4.752	-4.758	-2.040e-05	0.00219	0.04	0.021
sqr_000_05016	FeRu	2	-8.294	-8.563	-1.000e-06	0.00309	0.256	0.228
sqr_000_05018	NdTe	2	-5.006	-5.25	-1.000e-06	0.0011	0.444	0.47
sqr_000_05020	CoRh	2	-6.909	-7.011	-2.900e-05	0.00884	0.113	0.072
sqr_000_05026	PdYb	2	-3.898	-4.198	-5.900e-06	0.00031	0.379	0.177
sqr_000_05028	SnYb	2	-3.268	-3.28	4.500e-06	0.00699	0.137	0.163
sqr_000_05032	GeMnNi ₂	4	-5.735	-6.141	2.000e-06	0.00598	0.292	0.204
sqr_000_05033	TeYb	2	-3.674	-3.675	5.000e-07	0.00364	0.029	0.03
sqr_000_05036	GdZr	2	-6.185	-6.368	-1.900e-05	0.00305	0.465	0.455
sqr_000_05039	Co ₂ DyGa	4	-5.177	-5.54	-3.000e-06	0.0099	0.381	0.272
sqr_000_05041	HgTb	2	-2.842	-2.864	-4.000e-07	0.00065	0.193	0.165
sqr_000_05045	PdRu	2	-6.546	-6.947	-5.750e-04	0.00808	0.272	0.492
sqr_000_05046	GdZn	2	-3.19	-3.192	7.000e-07	0.00031	0.03	0.021
sqr_000_05047	GdGe	2	-5.151	-5.245	2.000e-06	0.00491	0.545	0.406
sqr_000_05051	DyPdSn	3	-4.92	-5.045	-5.000e-06	0.00545	0.403	0.522
sqr_000_05052	DyPd	2	-5.724	-5.763	-3.000e-06	0.00139	0.098	0.065
sqr_000_05055	AgNd	2	-3.957	-3.993	2.200e-06	0.00179	0.118	0.034
sqr_000_05056	EuTb	2	-2.923	-3.023	-1.190e-05	0.00272	0.244	0.209
sqr_000_05060	DyRh	2	-6.713	-6.767	-1.040e-03	0.00056	0.11	0.055
sqr_000_05061	DyU	2	-6.816	-7.248	-1.000e-06	0.00634	1.392	0.851
sqr_000_05062	PdYb	2	-3.894	-4.198	-2.460e-02	0.00449	0.38	0.36
sqr_000_05070	NiZr	2	-6.467	-7.302	-7.000e-06	0.007	0.746	0.753
sqr_000_05071	Pd ₂ SmYb	4	-4.876	-4.975	0.000e+00	0.00194	0.255	0.312
sqr_000_05075	DyZr	2	-6.243	-6.382	1.100e-05	0.00195	0.547	0.326
sqr_000_05078	ScTb	2	-5.319	-5.351	-7.000e-06	0.00203	0.431	0.344
sqr_000_05079	IrMn	2	-8.604	-9.024	-4.000e-06	0.00156	0.291	0.287
sqr_000_05081	HgYb	2	-1.345	-1.483	-1.000e-06	0.00054	0.301	0.202
sqr_000_05085	CoDy	2	-5.913	-5.92	-1.000e-06	0.00325	0.078	0.084
sqr_000_05088	DyGd	2	-4.009	-4.5	-1.000e-06	0.00209	0.396	0.72
sqr_000_05089	Be ₃ Mn	4	-4.83	-5.085	-2.000e-06	0.00289	0.316	0.213
sqr_000_05091	BeCo	2	-5.656	-5.699	7.000e-06	0.00334	0.108	0.062
sqr_000_05095	TbZn	2	-2.519	-3.186	-1.000e-06	0.0037	0.599	0.387
sqr_000_05098	HgNd	2	-2.847	-2.929	-3.300e-06	0.00249	0.178	0.073
sqr_000_05102	HoMgSmTb	4	-3.651	-3.791	-2.000e-06	0.002	0.348	0.192
sqr_000_05105	Yb ₂	2	-1.394	-1.459	-1.520e-05	0.00082	0.334	0.554
sqr_000_05106	Au ₂ GdLu	4	-4.73	-4.757	0.000e+00	0.00295	0.143	0.186
sqr_000_05108	NdRh	2	-6.577	-6.612	-2.600e-05	0.00203	0.094	0.068
sqr_000_05110	BeMn	2	-6.282	-6.284	-1.300e-05	0.00269	0.015	0.011
sqr_000_05114	GaGdLiSn	4	-3.3	-3.68	1.000e-06	0.00534	0.646	0.341
sqr_000_05115	PdTb	2	-5.709	-5.755	-1.000e-06	0.00082	0.201	0.23
sqr_000_05125	SeYb	2	-2.42	-4.572	-2.000e-07	0.00237	0.835	0.476
sqr_000_05127	TeYb	2	-3.608	-3.675	1.000e-07	0.00267	0.181	0.112
sqr_000_05129	GdYb	2	-2.77	-2.871	-2.000e-07	0.00138	0.234	0.124
sqr_000_05131	MnRu	2	-8.683	-8.974	-1.000e-06	0.00671	0.229	0.171
sqr_000_05134	GdSb	2	-5.058	-5.511	0.000e+00	0.00048	1.378	1.609
sqr_000_05137	NdRh	2	-6.574	-6.612	0.000e+00	0.00084	0.096	0.051
sqr_000_05140	Ag ₃ Nd	4	-3.406	-3.427	-3.000e-06	0.00724	0.439	0.32

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_05141	CeNd	2	-5.045	-5.197	-2.000e-06	0.00174	0.571	0.373
sqr_000_05143	DyRh	2	-6.716	-6.767	0.000e+00	0.00145	0.112	0.074
sqr_000_05145	TbZn	2	-3.181	-3.182	-9.600e-06	0.0028	0.022	0.02
sqr_000_05148	MnPt	2	-7.187	-7.548	-9.000e-06	0.00255	0.344	0.299
sqr_000_05150	GdZn	2	-3.187	-3.193	-4.900e-06	0.00241	0.046	0.054
sqr_000_05151	FePt	2	-6.93	-7.061	-4.000e-06	0.00261	0.104	0.069
sqr_000_05152	Co ₂	2	-6.462	-6.833	-1.900e-05	0.00777	0.348	0.513
sqr_000_05161	GdTe	2	-5.082	-5.086	-2.000e-06	0.00368	0.048	0.045
sqr_000_05164	SeTb	2	-5.302	-5.556	0.000e+00	0.00282	0.287	0.169
sqr_000_05169	DyTb	2	-3.938	-4.472	-6.800e-06	0.00128	0.418	0.749
sqr_000_05174	MnV	2	-9.245	-9.279	-8.000e-06	0.00569	0.101	0.082
sqr_000_05178	RuV	2	-9.29	-9.343	1.000e-06	0.0037	0.081	0.077
sqr_000_05183	AgTb	2	-3.944	-3.978	-1.500e-06	0.00763	0.112	0.106
sqr_000_05190	AlNdTiZn	4	-3.961	-4.397	-3.000e-06	0.00474	0.409	1.152
sqr_000_05192	CrMn	2	-9.018	-9.186	-3.000e-06	0.00874	0.33	0.232
sqr_000_05195	GdNi	2	-4.405	-5.374	-5.000e-06	0.00624	0.443	0.238
sqr_000_05197	SnYb	2	-3.264	-3.342	-4.400e-06	0.00659	0.492	0.353
sqr_000_05200	CoRu	2	-7.797	-7.951	8.000e-06	0.00428	0.204	0.242
sqr_000_05202	RuZn	2	-4.756	-4.985	0.000e+00	0.00323	0.174	0.124
sqr_000_05205	DyMg	2	-2.886	-3.097	7.000e-07	0.00423	0.295	0.195
sqr_000_05209	NdPd ₃	4	-5.64	-5.854	1.000e-06	0.00569	0.236	0.218
sqr_000_05211	AgDy	2	-3.947	-3.971	3.000e-07	0.00217	0.082	0.045
sqr_000_05212	AlNd	2	-4.563	-4.581	-1.600e-06	0.00356	0.084	0.07
sqr_000_05217	RhRu	2	-7.725	-8.125	-2.000e-06	0.00592	0.431	0.44
sqr_000_05219	MnNi	2	-6.854	-7.13	-3.170e-04	0.00428	0.324	0.408
sqr_000_05224	CoPt	2	-5.94	-6.484	-2.000e-06	0.00359	0.213	0.342
sqr_000_05226	NiTi	2	-6.996	-7.004	-3.000e-06	0.00186	0.065	0.054
sqr_000_05227	CuTb	2	-4.378	-4.395	-1.000e-06	0.00958	0.078	0.054
sqr_000_05230	HfRu	2	-9.717	-10.338	-1.000e-06	0.00764	0.484	0.325
sqr_000_05231	NiTi	2	-6.846	-6.977	1.100e-05	0.00136	0.329	0.192
sqr_000_05233	CdTb	2	-2.881	-2.974	-3.160e-05	0.00447	0.166	0.097
sqr_000_05238	MnZn	2	-4.545	-4.615	-1.000e-07	0.00513	0.106	0.07
sqr_000_05242	FeNi	2	-6.508	-6.639	2.000e-06	0.00723	0.139	0.147
sqr_000_05254	TbTl	2	-3.688	-3.765	-2.800e-06	0.00456	0.171	0.123
sqr_000_05258	GdHg	2	-2.868	-2.872	1.000e-07	0.00362	0.038	0.063
sqr_000_05259	CuGeTb	3	-4.722	-4.911	-1.060e-04	0.00801	0.301	0.207
sqr_000_05261	NdP	2	-6.086	-6.59	-5.000e-06	0.00242	1.328	1.183
sqr_000_05263	MgYb	2	-1.512	-1.526	-2.000e-06	0.00132	0.133	0.068
sqr_000_05265	BiNd	2	-5.077	-5.082	-1.000e-06	0.00306	0.407	0.183
sqr_000_05267	CoSi	2	-6.159	-6.625	-1.000e-06	0.00913	0.214	0.191
sqr_000_05268	NdSb	2	-5.302	-5.603	0.000e+00	0.00231	1.346	1.17
sqr_000_05270	NiV	2	-7.318	-7.408	0.000e+00	0.00724	0.121	0.086
sqr_000_05272	CuGd	2	-4.169	-4.196	-4.800e-06	0.00386	0.155	0.1
sqr_000_05273	MgNd	2	-3.177	-3.22	-2.000e-07	0.00089	0.388	0.338
sqr_000_05274	DyMg	2	-3.087	-3.103	4.000e-07	0.00175	0.094	0.058
sqr_000_05275	FePt	2	-6.637	-7.057	-3.000e-06	0.00234	0.183	0.149
sqr_000_05276	DyYb	2	-2.762	-2.826	-7.000e-07	0.00599	0.186	0.118
sqr_000_05282	C ₂ Mn	3	-7.451	-8.429	-3.000e-06	0.0053	0.417	0.447
sqr_000_05283	Ru ₂	2	-8.654	-9.089	-1.000e-06	0.00446	0.314	0.394
sqr_000_05285	RuTh	2	-8.307	-8.644	-1.400e-05	0.00256	0.357	0.245
sqr_000_05286	FeZn	2	-4.328	-4.342	-5.840e-05	0.00758	0.097	0.084
sqr_000_05288	RhRu	2	-7.829	-8.174	-5.000e-06	0.00305	0.319	0.326

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_05289	CoRu	2	-7.441	-7.938	0.000e+00	0.00444	0.25	0.258
sqr_000_05291	AlHfRu	3	-7.902	-8.172	-9.000e-06	0.00552	0.193	0.144
sqr_000_05293	NiPt	2	-5.729	-5.863	-1.000e-06	0.00105	0.274	0.394
sqr_000_05296	SbTb	2	-4.79	-5.492	2.000e-06	0.00367	1.443	0.899
sqr_000_05298	DyRh	2	-6.71	-6.767	-4.590e-04	0.00191	0.112	0.059
sqr_000_05300	NdRh	2	-6.581	-6.611	-9.000e-06	0.0036	0.083	0.046
sqr_000_05302	AgTb	2	-3.848	-3.98	-4.210e-05	0.00216	0.249	0.244
sqr_000_05303	SeTb	2	-5.544	-5.559	-1.000e-06	0.0018	0.077	0.06
sqr_000_05311	MnRhSi ₂	4	-1.574	-7.1	-1.000e-06	0.00572	0.616	0.528
sqr_000_05312	CoMn	2	-7.76	-7.958	-1.400e-05	0.00133	0.181	0.152
sqr_000_05314	DyNd	2	-4.471	-4.612	7.000e-07	0.00174	0.574	0.435
sqr_000_05316	AgDy	2	-3.97	-3.972	-8.000e-07	0.00105	0.024	0.027
sqr_000_05317	SmTbYYb	4	-2.516	-4.15	-2.000e-06	0.0031	0.914	0.6
sqr_000_05323	Mg ₃ Tb	4	-2.115	-2.327	-1.000e-06	0.00409	0.361	0.296
sqr_000_05327	P ₂ Tb	3	-4.808	-5.931	-3.000e-06	0.00421	0.857	2.327
sqr_000_05329	DyRh	2	-6.715	-6.767	5.000e-06	0.00631	0.104	0.07
sqr_000_05330	MgYb	2	-1.513	-1.526	1.540e-05	0.00069	0.133	0.096
sqr_000_05333	AuGdLi	3	-3.652	-3.769	0.000e+00	0.00205	0.186	0.225
sqr_000_05337	RuZn	2	-4.813	-5.003	1.000e-06	0.00208	0.173	0.134
sqr_000_05341	NdPaThZn	4	-5.423	-5.521	-2.000e-06	0.004	0.236	0.157
sqr_000_05344	PdTb	2	-5.749	-5.757	-4.000e-06	0.00257	0.043	0.024
sqr_000_05346	HgTb	2	-2.856	-2.864	1.200e-06	0.00048	0.069	0.044
sqr_000_05350	NdOsRhSn	4	-5.567	-6.864	-7.000e-06	0.00499	0.439	0.584
sqr_000_05351	GdHg	2	-2.841	-2.873	-3.000e-07	0.00092	0.098	0.067
sqr_000_05355	GdIn	2	-4.025	-4.076	-6.700e-06	0.00302	0.138	0.081
sqr_000_05356	CDy	2	-6.309	-6.468	-6.000e-06	0.00302	0.293	0.212
sqr_000_05357	Ru ₂	2	-8.467	-9.109	2.800e-05	0.00179	0.471	0.385
sqr_000_05359	MoRu	2	-9.719	-9.963	1.000e-06	0.00218	0.323	0.27
sqr_000_05367	CdNd	2	-3.003	-3.057	-6.100e-06	0.00534	0.151	0.078
sqr_000_05370	TbZn	2	-3.112	-3.18	-7.300e-06	0.00234	0.161	0.099
sqr_000_05371	FeHf	2	-9.356	-9.416	-5.000e-06	0.00208	0.171	0.099
sqr_000_05373	CuGd	2	-4.338	-4.393	0.000e+00	0.00223	0.206	0.189
sqr_000_05375	AlRu	2	-6.753	-7.113	-1.000e-06	0.0011	0.199	0.166
sqr_000_05376	SnYb	2	-2.889	-3.3	-2.100e-06	0.00175	0.536	0.598
sqr_000_05382	NiV	2	-7.294	-7.407	-1.200e-05	0.0049	0.133	0.141
sqr_000_05383	AuSiTb	3	-4.732	-5.227	-6.000e-06	0.00819	0.847	0.911
sqr_000_05391	NdSe	2	-5.558	-5.732	0.000e+00	0.00083	0.382	0.354
sqr_000_05393	AgHgYb	3	-1.874	-1.93	4.000e-07	0.00225	0.308	0.177
sqr_000_05394	YbZn	2	-1.516	-1.625	2.000e-06	0.00274	0.274	0.208
sqr_000_05397	GdSi	2	-5.301	-5.509	1.000e-06	0.00061	0.504	0.346
sqr_000_05404	CdGd	2	-2.987	-2.993	5.000e-07	0.00355	0.035	0.027
sqr_000_05406	InYb	2	-2.514	-2.527	-1.000e-06	0.00122	0.087	0.062
sqr_000_05410	FePTb	3	-4.465	-6.419	0.000e+00	0.006	0.937	0.983
sqr_000_05414	GdHg	2	-2.753	-2.884	2.880e-05	0.00554	0.224	0.139
sqr_000_05416	GdTe	2	-4.594	-5.09	0.000e+00	0.00502	0.453	0.343
sqr_000_05421	MgTb	2	-3.069	-3.122	-1.000e-07	0.00181	0.416	0.312
sqr_000_05423	TbTe	2	-4.93	-5.038	1.000e-06	0.00966	0.213	0.13
sqr_000_05425	Al ₂ AuNd	4	-3.837	-4.282	0.000e+00	0.00684	0.362	0.368
sqr_000_05427	InYb	2	-2.512	-2.527	-3.600e-06	0.00415	0.093	0.053
sqr_000_05430	LiRu	2	-4.945	-5.374	-2.000e-06	0.00529	0.85	0.567
sqr_000_05431	GdPdSn	3	-5.131	-5.19	0.000e+00	0.00337	0.208	0.143
sqr_000_05432	FeRu	2	-8.415	-8.561	-1.600e-05	0.00225	0.175	0.191

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_05435	TlYb	2	-2.266	-2.35	-4.000e-07	0.00098	0.24	0.11
sqr_000_05437	MgTb	2	-3.107	-3.122	-1.900e-06	0.00052	0.087	0.05
sqr_000_05441	AlYb	2	-2.742	-2.793	1.500e-06	0.00223	0.167	0.105
sqr_000_05442	NdRh	2	-6.326	-6.613	2.000e-06	0.00123	0.377	0.243
sqr_000_05445	AlCo	2	-5.722	-5.987	1.000e-06	0.00178	0.47	0.639
sqr_000_05448	CoMn	2	-7.601	-7.96	0.000e+00	0.00199	0.245	0.27
sqr_000_05453	RuV	2	-9.168	-9.323	-1.000e-06	0.00469	0.216	0.14
sqr_000_05456	NdPd ₃	4	-5.719	-5.856	-1.000e-06	0.00286	0.174	0.113
sqr_000_05457	AgIrRuTb	4	-6.376	-6.38	-2.000e-06	0.00474	0.044	0.047
sqr_000_05461	PdRu	2	-6.314	-6.945	-3.000e-06	0.00471	0.571	0.418
sqr_000_05464	CoRu	2	-7.607	-7.952	-1.600e-05	0.00952	0.339	0.212
sqr_000_05465	GdYb	2	-2.863	-2.877	-5.000e-06	0.00145	0.089	0.08
sqr_000_05467	GdSb	2	-5.033	-5.52	-1.000e-06	0.00314	1.44	0.774
sqr_000_05469	NdP	2	-6.088	-6.589	-1.000e-06	0.00547	1.346	1.186
sqr_000_05471	CdYb	2	-1.394	-1.522	-4.400e-06	0.00226	0.307	0.253
sqr_000_05475	AlRu	2	-6.532	-7.108	0.000e+00	0.00395	0.216	0.128
sqr_000_05477	GaRu	2	-6.333	-6.338	-3.000e-06	0.00089	0.025	0.014
sqr_000_05478	GdSb	2	-5.187	-5.512	0.000e+00	0.00607	1.45	1.485
sqr_000_05479	Yb ₂	2	-1.291	-1.446	-1.000e-06	0.00054	0.351	0.241
sqr_000_05480	BeMn	2	-6.136	-6.323	0.000e+00	0.00378	0.174	0.149
sqr_000_05483	NiTi	2	-6.757	-6.978	1.000e-05	0.00404	0.379	0.337
sqr_000_05484	GdNd	2	-4.25	-4.639	-1.600e-06	0.00035	0.531	0.573
sqr_000_05488	STb	2	-5.939	-6.008	-1.700e-05	0.00158	0.139	0.121
sqr_000_05499	CoSi	2	-6.4	-6.626	1.000e-06	0.00115	0.162	0.105
sqr_000_05504	InNd	2	-4.27	-3.717	-1.649e-04	0.00285	0.208	0.212
sqr_000_05507	SYb	2	-4.183	-4.728	-1.900e-06	0.00302	0.513	0.403
sqr_000_05508	NiRu	2	-7.102	-7.181	-3.000e-06	0.00328	0.225	0.294
sqr_000_05511	AgYb	2	-2.451	-2.525	-2.300e-06	0.00178	0.218	0.137
sqr_000_05512	GdIn	2	-4.032	-4.068	-2.700e-06	0.00122	0.14	0.193
sqr_000_05515	ErNi	2	-5.4	-5.419	-1.900e-05	0.00641	0.088	0.102
sqr_000_05516	DyZn	2	-3.171	-3.172	9.000e-07	0.00072	0.027	0.019
sqr_000_05518	GdIn ₂ Mg	4	-3.056	-3.23	2.000e-06	0.00705	0.306	0.151
sqr_000_05522	AlDyPtRh	4	-5.132	-6.241	1.000e-06	0.00127	0.387	0.438
sqr_000_05526	PtTb	2	-6.48	-6.522	-4.000e-06	0.00341	0.092	0.063
sqr_000_05527	PaPdYbZr	4	-6.041	-6.237	-3.000e-06	0.00359	0.878	0.935
sqr_000_05528	DyPb	2	-4.557	-4.484	-7.000e-07	0.00293	0.446	0.343
sqr_000_05532	MnNi ₃	4	-0.554	-6.117	6.000e-06	0.00331	0.631	0.346
sqr_000_05535	MgTb	2	-3.078	-3.122	-8.500e-06	0.00062	0.151	0.106
sqr_000_05536	CuFe	2	-5.403	-5.536	-4.000e-06	0.00229	0.352	0.39
sqr_000_05538	NiV	2	-7.332	-7.418	-2.800e-05	0.00402	0.164	0.18
sqr_000_05545	PdTb	2	-5.672	-5.756	2.000e-06	0.00241	0.261	0.165
sqr_000_05548	GaRu	2	-5.883	-6.318	1.000e-06	0.00324	0.314	0.191
sqr_000_05552	AgTb	2	-3.832	-3.98	3.600e-06	0.00077	0.237	0.144
sqr_000_05559	GdHg	2	-2.872	-2.873	-1.600e-06	0.00066	0.022	0.02
sqr_000_05562	CoHo	2	-5.845	-5.925	-1.780e-04	0.00562	0.14	0.042
sqr_000_05564	AuRu	2	-5.551	-5.642	-2.600e-05	0.00497	0.108	0.06
sqr_000_05566	InRu	2	-5.471	-5.731	0.000e+00	0.00299	0.478	0.513
sqr_000_05584	NdSi ₂	3	-5.667	-5.756	4.000e-06	0.00217	0.163	0.161
sqr_000_05586	Co ₂	2	-6.458	-6.833	0.000e+00	0.00489	0.354	0.491
sqr_000_05587	AgDy	2	-3.944	-3.969	-4.000e-07	0.00061	0.088	0.081
sqr_000_05595	CdNd	2	-3.015	-3.046	0.000e+00	0.00394	0.102	0.044
sqr_000_05597	RuU	2	-10.176	-10.251	-1.600e-05	0.0068	0.106	0.069

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_05599	CdYb	2	-1.448	-1.521	3.000e-07	0.00406	0.219	0.157
sqr_000_05603	Be ₃ Mn	4	-4.192	-5.208	-1.000e-06	0.00425	0.421	0.321
sqr_000_05604	DyRh ₃	4	-6.085	-7.016	0.000e+00	0.00319	0.325	0.269
sqr_000_05608	NbRu	2	-9.752	-9.905	-2.000e-05	0.00262	0.152	0.206
sqr_000_05610	CdGd	2	-2.975	-2.993	2.500e-06	0.00213	0.075	0.057
sqr_000_05614	FeRu	2	-8.255	-8.551	0.000e+00	0.00392	0.382	0.328
sqr_000_05623	Pt ₃ Yb	4	-5.621	-5.734	0.000e+00	0.0028	0.148	0.126
sqr_000_05624	NiV	2	-6.916	-7.369	-2.000e-06	0.00394	0.324	0.315
sqr_000_05628	RuY	2	-7.85	-8.084	-3.800e-05	0.00079	0.181	0.127
sqr_000_05629	GaHoTb	3	-3.349	-4.211	1.000e-06	0.00687	0.733	0.413
sqr_000_05635	TeYb	2	-3.673	-3.962	0.000e+00	0.00185	1.464	1.141
sqr_000_05637	DyPt	2	-6.511	-6.53	-1.000e-06	0.00476	0.072	0.026
sqr_000_05638	F ₃ Ru	4	-3.598	-4.977	1.000e-06	0.00687	0.367	0.177
sqr_000_05643	SbTb	2	-5.129	-5.49	0.000e+00	0.00066	1.382	1.313
sqr_000_05644	GdSi	2	-5.394	-5.508	-7.000e-06	0.00699	0.441	0.423
sqr_000_05645	PdTb	2	-5.637	-5.753	-6.000e-06	0.00075	0.174	0.106
sqr_000_05646	GdIr ₃	4	-7.179	-8.123	-3.000e-06	0.00669	0.325	1.131
sqr_000_05652	MnRu	2	-8.587	-8.968	1.400e-05	0.00127	0.171	0.273
sqr_000_05654	MnPt	2	-7.009	-7.543	1.000e-06	0.0015	0.372	0.48
sqr_000_05655	RuSc	2	-8.116	-8.228	-3.000e-06	0.0017	0.16	0.075
sqr_000_05659	EuTb	2	-3.061	-3.067	2.000e-06	0.00212	0.1	0.092
sqr_000_05663	SbTb	2	-5.126	-5.484	-5.000e-06	0.00083	1.393	1.318
sqr_000_05666	FeNi	2	-6.575	-6.637	-5.000e-06	0.00844	0.101	0.069
sqr_000_05669	NiTc	2	-7.777	-7.887	-4.000e-06	0.00298	0.153	0.133
sqr_000_05670	MnRu	2	-8.737	-8.98	0.000e+00	0.00621	0.388	0.322
sqr_000_05675	GdYb	2	-2.803	-2.873	-3.300e-06	0.00058	0.194	0.136
sqr_000_05676	TbZn	2	-2.791	-3.182	-9.600e-06	0.00285	0.425	0.267
sqr_000_05681	Ru ₂	2	-8.585	-9.075	-4.000e-06	0.00436	0.306	0.273
sqr_000_05682	NdTb	2	-4.212	-4.625	-8.000e-07	0.00474	0.492	0.39
sqr_000_05684	DyPd	2	-5.542	-5.758	-2.000e-06	0.00645	0.243	0.142
sqr_000_05687	NdYb	2	-2.64	-2.988	-3.500e-06	0.00238	0.433	0.257
sqr_000_05693	STb	2	-5.949	-6.008	-1.000e-06	0.00072	0.154	0.1
sqr_000_05694	NdTe	2	-5.24	-5.248	-1.000e-06	0.00376	0.051	0.037
sqr_000_05695	RuSm	2	-6.38	-7.03	-1.000e-06	0.00297	0.309	0.181
sqr_000_05696	CaYb	2	-1.51	-1.678	-3.030e-05	0.00165	0.424	0.856
sqr_000_05702	CMn	2	-8.2	-9.039	1.000e-06	0.00299	0.518	0.65
sqr_000_05713	MnTa	2	-10.297	-10.65	-1.000e-06	0.00112	0.172	0.096
sqr_000_05716	GaLuNd	3	-3.76	-4.294	1.000e-06	0.00784	0.874	0.836
sqr_000_05718	ScTb	2	-5.243	-5.347	-2.000e-06	0.00592	0.303	0.414
sqr_000_05723	CoDyFeNi	4	-5.809	-6.089	-1.000e-06	0.00834	0.268	0.24
sqr_000_05725	HgNd	2	-2.886	-2.916	-2.000e-06	0.00125	0.097	0.071
sqr_000_05726	RuZr	2	-9.497	-9.521	-2.000e-06	0.00569	0.088	0.084
sqr_000_05728	NdYb	2	-2.772	-2.993	0.000e+00	0.00053	0.35	0.176
sqr_000_05729	MgNd	2	-3.132	-3.22	0.000e+00	0.00331	0.193	0.128
sqr_000_05730	DyNd	2	-4.123	-4.604	1.000e-06	0.00209	0.491	0.365
sqr_000_05731	MgRu	2	-5.066	-5.119	-3.000e-06	0.00437	0.108	0.06
sqr_000_05740	GePrYbZr	4	-4.95	-4.981	-2.000e-06	0.00337	0.167	0.166
sqr_000_05742	DyPb	2	-4.345	-4.47	-1.930e-05	0.00187	0.296	0.32
sqr_000_05744	DyTe	2	-4.405	-5.0	1.400e-06	0.00448	0.536	0.481
sqr_000_05745	HgYb	2	-1.352	-1.483	1.000e-07	0.00486	0.298	0.176
sqr_000_05747	PtTb	2	-6.426	-6.524	-1.000e-06	0.00381	0.172	0.124
sqr_000_05752	FeNi	2	-6.58	-6.636	1.000e-06	0.00279	0.129	0.096

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_05755	MnPd	2	-6.445	-6.811	-6.400e-05	0.0056	0.422	0.529
sqr_000_05756	GdGe ₂ Tm	4	-5.235	-5.38	-1.600e-05	0.00798	0.254	0.2
sqr_000_05761	DySc	2	-5.215	-5.329	0.000e+00	0.00201	0.322	0.398
sqr_000_05765	FePt	2	-6.924	-7.063	-7.200e-05	0.00462	0.196	0.157
sqr_000_05766	MgTb	2	-3.096	-3.122	-6.000e-07	0.0006	0.119	0.09
sqr_000_05770	GdPtSiZr	4	-6.043	-6.962	-1.000e-06	0.00498	0.682	1.588
sqr_000_05779	MnPd	2	-6.547	-6.804	-1.000e-05	0.00336	0.499	0.319
sqr_000_05782	Ru ₂	2	-8.435	-9.113	0.000e+00	0.00817	0.479	0.29
sqr_000_05783	HfRu	2	-10.139	-10.374	-4.000e-06	0.0014	0.239	0.167
sqr_000_05793	CoFeNiSi	4	-6.434	-6.637	-1.000e-06	0.00628	0.471	0.597
sqr_000_05794	MgYb	2	-1.517	-1.529	-1.310e-05	0.00266	0.167	0.149
sqr_000_05796	GdSe	2	-4.982	-5.597	-5.000e-06	0.00145	0.49	0.239
sqr_000_05800	TbTl	2	-3.452	-3.762	-9.000e-07	0.00105	0.389	0.229
sqr_000_05802	CdCeDy	3	-3.745	-3.831	-1.100e-05	0.00865	0.763	0.655
sqr_000_05806	CrMn	2	-9.047	-9.187	-1.300e-05	0.00538	0.321	0.358
sqr_000_05807	MnNb	2	-8.51	-9.706	-3.100e-05	0.00424	0.402	0.187
sqr_000_05810	GdSe	2	-5.294	-5.596	-3.300e-05	0.0013	0.404	0.347
sqr_000_05815	CoNi	2	-6.056	-6.072	1.000e-06	0.00039	0.046	0.04
sqr_000_05816	TbTl	2	-3.152	-3.772	-3.000e-07	0.00348	0.581	0.493
sqr_000_05818	NiTi	2	-6.751	-6.971	-8.000e-06	0.00511	0.373	0.287
sqr_000_05820	TeYb	2	-3.289	-3.971	-1.000e-06	0.00243	1.481	1.379
sqr_000_05825	HgYb	2	-1.431	-1.477	-2.600e-06	0.00162	0.169	0.109
sqr_000_05826	DyNi	2	-5.323	-5.407	-3.000e-06	0.00446	0.154	0.106
sqr_000_05827	AuMn	2	-5.236	-5.539	-2.000e-06	0.00181	0.471	0.678
sqr_000_05833	DyRu	2	-7.157	-7.172	1.500e-05	0.00801	0.064	0.063
sqr_000_05844	RuZr	2	-9.074	-9.505	-5.000e-06	0.00539	0.427	0.264
sqr_000_05845	MgNd	2	-3.186	-3.217	-1.170e-05	0.00123	0.124	0.087
sqr_000_05848	NdTl	2	-3.843	-3.869	4.000e-07	0.00068	0.183	0.179
sqr_000_05849	CoPt	2	-6.109	-6.489	2.000e-06	0.00466	0.45	0.184
sqr_000_05850	GdZn	2	-3.138	-3.191	-1.120e-05	0.00089	0.145	0.083
sqr_000_05854	HgTb	2	-2.859	-2.864	6.000e-07	0.00061	0.044	0.01
sqr_000_05863	LuTb	2	-4.373	-4.46	2.260e-05	0.00994	0.563	0.458
sqr_000_05866	AlFe	2	-5.986	-6.3	-3.000e-06	0.00436	0.549	0.744
sqr_000_05873	NiZn	2	-3.373	-3.546	-1.200e-06	0.00386	0.312	0.22
sqr_000_05875	CdYb	2	-1.379	-1.523	-8.000e-06	0.00235	0.335	0.239
sqr_000_05877	NaNd	2	-2.391	-2.668	-1.500e-06	0.00637	0.547	0.65
sqr_000_05878	RuSc	2	-8.069	-8.226	-2.000e-05	0.00175	0.213	0.181
sqr_000_05880	DySn	2	-4.66	-4.813	-1.200e-06	0.00603	0.322	0.455
sqr_000_05881	CdNd	2	-2.939	-3.043	-3.000e-07	0.0021	0.183	0.11
sqr_000_05891	DyRh	2	-6.711	-6.768	1.900e-05	0.007	0.134	0.121
sqr_000_05895	DyTl	2	-3.677	-3.735	1.000e-06	0.0009	0.189	0.155
sqr_000_05897	FeIr ₂ Os	4	-8.961	-9.233	-3.000e-06	0.00459	0.344	0.412
sqr_000_05898	NiPd	2	-5.091	-5.267	-9.000e-06	0.00646	0.205	0.101
sqr_000_05900	FePt	2	-6.851	-7.062	-2.100e-05	0.00522	0.251	0.334
sqr_000_05901	MnPt	2	-7.439	-7.549	-1.000e-05	0.00199	0.168	0.155
sqr_000_05903	GdSe	2	-5.594	-5.6	-5.000e-06	0.00235	0.04	0.027
sqr_000_05905	AuNd	2	-4.746	-4.751	-3.600e-06	0.004	0.046	0.025
sqr_000_05906	DyPd	2	-5.751	-5.763	-3.000e-06	0.00326	0.054	0.032
sqr_000_05908	BiGdPd	3	-4.763	-5.133	-1.000e-05	0.00656	0.435	0.704
sqr_000_05914	AlRu	2	-7.105	-7.131	-1.000e-06	0.00303	0.078	0.062
sqr_000_05917	GdTe	2	-4.889	-5.088	-2.400e-05	0.00479	0.266	0.186
sqr_000_05918	SbTb	2	-5.159	-5.485	-1.000e-06	0.00101	1.422	1.129

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_05921	AgDy	2	-3.54	-3.98	-7.000e-07	0.00076	0.432	0.232
sqr_000_05924	NdTb	2	-4.078	-4.62	-2.500e-06	0.00176	0.488	0.327
sqr_000_05927	CaNd	2	-2.83	-3.199	3.200e-06	0.00157	0.438	0.347
sqr_000_05939	RuZr	2	-8.908	-9.519	-4.000e-06	0.00461	0.545	0.706
sqr_000_05946	NdTl	2	-3.865	-3.868	-4.400e-06	0.00134	0.051	0.047
sqr_000_05948	NiZn	2	-3.321	-3.549	8.000e-07	0.00257	0.299	0.233
sqr_000_05950	GdSb	2	-5.041	-5.5	-2.000e-06	0.00084	1.456	0.863
sqr_000_05953	DyIn	2	-4.019	-4.023	-2.100e-06	0.00075	0.045	0.037
sqr_000_05954	MnV	2	-9.119	-9.277	-5.200e-05	0.00222	0.184	0.136
sqr_000_05956	BeFe	2	-6.024	-6.029	-7.000e-06	0.00147	0.044	0.052
sqr_000_05957	AgDy	2	-3.963	-3.972	-1.200e-06	0.00131	0.052	0.024
sqr_000_05963	CuTb	2	-4.38	-4.395	-2.700e-06	0.00404	0.067	0.049
sqr_000_05969	RuSe ₂	3	-5.028	-5.525	-3.000e-06	0.00632	0.781	0.383
sqr_000_05977	RuU	2	-10.184	-10.315	-5.000e-06	0.0011	0.449	0.349
sqr_000_05979	NiRu	2	-6.882	-7.174	-9.000e-06	0.00283	0.359	0.345
sqr_000_05981	TlYb	2	-2.335	-2.341	-3.600e-06	0.00144	0.067	0.045
sqr_000_05983	Be ₃ Ni	4	-3.177	-4.468	0.0000e+00	0.00473	0.723	0.524
sqr_000_05984	MgNd	2	-3.103	-3.219	-4.000e-07	0.00081	0.219	0.119
sqr_000_05985	EuNd	2	-3.124	-3.151	-1.000e-06	0.00253	0.139	0.095
sqr_000_05987	BeFe	2	-5.898	-6.031	-2.000e-05	0.00355	0.201	0.148
sqr_000_05989	GdSe	2	-5.472	-5.596	0.0000e+00	0.00222	0.193	0.141
sqr_000_05993	TbZn	2	-3.176	-3.183	-2.700e-06	0.0047	0.065	0.051
sqr_000_05998	PtRu	2	-7.114	-7.617	-1.000e-05	0.00351	0.366	0.171
sqr_000_06001	BiDy	2	-4.753	-4.879	9.0000e-07	0.00139	0.59	0.406
sqr_000_06007	CoLiTb	3	-4.035	-4.342	4.000e-06	0.00158	0.841	0.886
sqr_000_06027	AgYb	2	-2.264	-2.532	-7.000e-07	0.00277	0.446	0.199
sqr_000_06028	AlNi	2	-4.99	-5.263	-1.000e-06	0.00262	0.446	0.313
sqr_000_06030	GdSc	2	-5.322	-5.366	-1.000e-05	0.00243	0.369	0.34
sqr_000_06034	DyTl	2	-3.721	-3.732	-1.700e-06	0.00158	0.06	0.045
sqr_000_06040	CoNi	2	-5.919	-6.064	-1.700e-04	0.00978	0.317	0.382
sqr_000_06041	TbTl	2	-3.664	-3.763	-2.400e-06	0.00299	0.212	0.154
sqr_000_06042	NdSe	2	-5.712	-5.737	-4.000e-06	0.00368	0.136	0.138
sqr_000_06046	CuGd	2	-4.37	-4.393	-2.850e-05	0.00102	0.096	0.035
sqr_000_06051	RhRu ₂	3	-7.912	-8.425	-2.100e-05	0.00865	0.415	0.132
sqr_000_06053	FeTa	2	-10.023	-10.119	-3.000e-05	0.00203	0.183	0.1
sqr_000_06054	DyGd	2	-4.304	-4.525	-3.100e-06	0.00049	0.326	0.465
sqr_000_06057	PbS ₂ Tb	4	-5.791	-5.224	-1.600e-05	0.00726	0.132	1.103
sqr_000_06058	GdMg	2	-3.122	-3.141	-1.400e-06	0.00237	0.096	0.071
sqr_000_06059	GdRh	2	-6.296	-6.722	3.000e-06	0.0002	0.332	0.244
sqr_000_06066	Ni ₂	2	-5.405	-5.41	9.000e-06	0.00097	0.046	0.054
sqr_000_06068	BeCo	2	-5.69	-5.7	-1.000e-06	0.00308	0.051	0.039
sqr_000_06070	NiV	2	-7.234	-7.411	-1.000e-06	0.00289	0.368	0.476
sqr_000_06072	CoNd	2	-5.697	-5.793	-1.000e-06	0.00925	0.184	0.154
sqr_000_06073	TlYb	2	-2.32	-2.342	1.000e-07	0.00158	0.165	0.168
sqr_000_06074	Ag ₂ DyW	4	-5.044	-5.257	1.000e-06	0.00407	0.222	0.204
sqr_000_06076	CdDy	2	-2.873	-2.96	-9.000e-06	0.00564	0.155	0.086
sqr_000_06084	MgYb	2	-1.475	-1.526	0.0000e+00	0.00154	0.226	0.148
sqr_000_06085	FeNi	2	-6.185	-6.641	-1.000e-06	0.00099	0.546	0.356
sqr_000_06092	TbTe	2	-4.973	-5.04	-1.000e-06	0.00298	0.286	0.215
sqr_000_06094	GdS	2	-5.95	-6.044	-3.000e-06	0.00132	0.258	0.219
sqr_000_06095	DyYb	2	-2.77	-2.826	2.000e-07	0.00196	0.173	0.122
sqr_000_06098	NdSn	2	-4.761	-4.954	-1.000e-07	0.00095	0.487	0.472

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_06102	MnNi	2	-6.858	-7.106	1.000e-06	0.00843	0.49	0.506
sqr_000_06108	AlRu	2	-6.745	-7.116	-3.000e-06	0.00314	0.255	0.152
sqr_000_06117	TbZr	2	-6.251	-6.38	0.000e+00	0.00066	0.528	0.354
sqr_000_06118	TlYb	2	-2.324	-2.341	-1.300e-06	0.00078	0.135	0.083
sqr_000_06124	FeZn	2	-4.213	-4.344	-1.400e-06	0.00056	0.227	0.171
sqr_000_06125	GdMg	2	-3.113	-3.141	-5.700e-06	0.00161	0.114	0.067
sqr_000_06127	Fe ₂	2	-7.969	-8.077	-6.000e-06	0.00452	0.182	0.155
sqr_000_06133	PtTb	2	-6.469	-6.523	0.000e+00	0.00108	0.11	0.071
sqr_000_06134	NdSm ₃	4	-4.415	-4.65	-5.000e-06	0.00187	0.386	0.383
sqr_000_06135	NdYb	2	-2.931	-2.994	-1.960e-05	0.00053	0.194	0.146
sqr_000_06138	GdIn	2	-4.062	-4.069	-1.200e-06	0.00217	0.05	0.047
sqr_000_06143	MnNb	2	-9.725	-9.737	-1.300e-05	0.00312	0.072	0.082
sqr_000_06144	DyOsRhRu	4	-6.8	-7.965	-8.000e-06	0.00988	0.349	0.265
sqr_000_06145	NiRu	2	-6.989	-7.207	-4.000e-06	0.0081	0.473	0.559
sqr_000_06146	AlNd	2	-4.56	-4.578	-3.000e-07	0.00166	0.079	0.047
sqr_000_06147	NiSc	2	-5.532	-6.313	-7.000e-06	0.00509	0.641	0.467
sqr_000_06155	AsNd	2	-5.575	-6.19	-5.000e-06	0.00318	1.296	1.054
sqr_000_06158	CrMn	2	-8.952	-9.181	5.000e-06	0.00544	0.216	1.506
sqr_000_06159	MnZn	2	-4.619	-4.796	8.300e-06	0.00629	0.372	0.153
sqr_000_06160	NiZr	2	-7.087	-7.347	-7.000e-06	0.00564	0.564	0.28
sqr_000_06165	DyPr	2	-4.394	-4.613	4.000e-07	0.00111	0.356	0.488
sqr_000_06166	NdRh	2	-6.579	-6.612	-3.000e-06	0.00365	0.086	0.06
sqr_000_06167	DyYb	2	-2.684	-2.821	-3.900e-06	0.00099	0.266	0.121
sqr_000_06169	GdSb	2	-5.189	-5.512	-1.000e-05	0.00225	1.443	0.44
sqr_000_06176	CoDy	2	-5.793	-5.923	-6.100e-05	0.00276	0.19	0.118
sqr_000_06178	RhRu	2	-7.74	-8.146	-1.100e-05	0.00672	0.299	0.323
sqr_000_06191	CdNd	2	-2.969	-3.044	-9.400e-06	0.00182	0.151	0.083
sqr_000_06192	AgDy	2	-3.954	-3.971	-3.200e-06	0.00183	0.066	0.041
sqr_000_06193	CoPt	2	-6.287	-6.488	2.000e-06	0.00488	0.202	0.183
sqr_000_06203	MgNd	2	-3.171	-3.22	-1.900e-06	0.00088	0.222	0.133
sqr_000_06204	RuTc	2	-9.332	-9.733	-1.000e-06	0.00259	0.165	0.266
sqr_000_06206	DyHg	2	-2.754	-2.849	-7.000e-06	0.00087	0.155	0.095
sqr_000_06207	Al ₂ FeMn	4	-6.293	-6.378	1.000e-06	0.00513	0.166	0.146
sqr_000_06210	Ru ₂	2	-8.689	-9.11	-5.000e-06	0.00244	0.166	0.299
sqr_000_06211	ErFe	2	-5.122	-6.15	-7.000e-05	0.00025	0.728	0.403
sqr_000_06213	AgGd	2	-3.973	-3.983	-3.570e-05	0.003	0.053	0.029
sqr_000_06219	AlDy	2	-4.524	-4.539	-6.300e-06	0.00392	0.071	0.059
sqr_000_06224	MgNd	2	-3.154	-3.22	1.300e-06	0.00196	0.199	0.099
sqr_000_06226	CoNi	2	-5.933	-6.073	-3.200e-05	0.00309	0.202	0.224
sqr_000_06227	InNi	2	-3.204	-4.075	-2.100e-05	0.00615	0.674	0.335
sqr_000_06228	NdTe	2	-5.233	-5.248	-3.000e-06	0.00392	0.079	0.06
sqr_000_06231	AsNd	2	-5.761	-6.157	-1.000e-06	0.00242	1.336	0.577
sqr_000_06232	GdHg	2	-2.83	-2.872	2.000e-07	0.00142	0.118	0.085
sqr_000_06233	RuV	2	-9.273	-9.333	-4.000e-06	0.006	0.124	0.114
sqr_000_06234	NdRh	2	-6.274	-6.608	0.000e+00	0.00153	0.306	0.165
sqr_000_06235	GdTm	2	-4.163	-4.478	-1.437e-04	0.00429	0.392	0.624
sqr_000_06236	AuSiTb ₂	4	-4.946	-5.254	-1.000e-06	0.00596	0.265	0.324
sqr_000_06238	FeSi	2	-7.068	-7.319	-3.400e-05	0.00421	0.36	0.378
sqr_000_06241	AlDy	2	-4.521	-4.539	-3.000e-07	0.00289	0.086	0.098
sqr_000_06244	InTb	2	-4.041	-4.049	-2.880e-05	0.00341	0.102	0.071
sqr_000_06247	NdPb ₃	4	-3.865	-4.212	-2.000e-06	0.00473	0.469	0.393
sqr_000_06249	IrRu	2	-8.857	-9.081	0.000e+00	0.00411	0.176	0.144

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_06250	AgGd	2	-3.973	-3.983	-1.900e-06	0.00131	0.057	0.038
sqr_000_06253	RhSi ₂ Tb	4	-4.786	-6.128	-1.000e-06	0.00461	0.539	0.654
sqr_000_06255	PtRu	2	-7.558	-7.589	0.000e+00	0.00221	0.076	0.05
sqr_000_06258	NdZn	2	-3.207	-3.221	-1.050e-05	0.00097	0.083	0.08
sqr_000_06260	RhRu	2	-7.706	-8.149	-1.400e-05	0.00985	0.445	0.332
sqr_000_06261	HgNd	2	-2.546	-2.943	9.000e-07	0.0022	0.435	0.263
sqr_000_06262	AsNd	2	-5.589	-6.184	1.000e-06	0.00167	1.348	0.685
sqr_000_06263	AlTb	2	-4.542	-4.55	0.000e+00	0.00139	0.06	0.056
sqr_000_06268	GdZn	2	-3.189	-3.192	-2.500e-06	0.00158	0.043	0.051
sqr_000_06274	MnPd	2	-6.617	-6.815	0.000e+00	0.00174	0.241	0.134
sqr_000_06277	BiDy	2	-4.788	-4.889	-6.000e-07	0.00368	0.497	0.214
sqr_000_06283	DyOs	2	-7.838	-7.917	-2.000e-06	0.00287	0.125	0.107
sqr_000_06285	CdYb	2	-1.495	-1.518	1.300e-06	0.00188	0.114	0.105
sqr_000_06289	DySmZn	3	-3.122	-3.459	1.000e-06	0.00957	0.619	0.518
sqr_000_06291	TbTl	2	-3.741	-3.755	-1.300e-06	0.00102	0.072	0.048
sqr_000_06292	AuGd	2	-4.751	-4.767	-6.000e-07	0.00342	0.069	0.038
sqr_000_06294	AlDy	2	-4.357	-4.54	-2.000e-07	0.00123	0.265	0.18
sqr_000_06303	AgNiZn	3	-2.896	-3.129	1.300e-06	0.0037	0.521	0.458
sqr_000_06304	DySiTb	3	-4.315	-5.032	-4.000e-06	0.00477	0.426	0.395
sqr_000_06305	NdZr	2	-6.301	-6.395	-3.000e-06	0.00241	0.64	0.597
sqr_000_06307	FeNi	2	-6.599	-6.637	-8.300e-05	0.00367	0.13	0.178
sqr_000_06309	GdS	2	-5.488	-6.038	0.000e+00	0.00088	0.458	0.253
sqr_000_06310	DyHg	2	-2.515	-2.867	-2.000e-06	0.00117	0.379	0.277
sqr_000_06317	MnRu	2	-8.469	-8.967	-3.000e-06	0.00155	0.264	0.398
sqr_000_06318	AuYb	2	-3.144	-3.322	-2.900e-06	0.00265	0.289	0.186
sqr_000_06322	DyMg	2	-3.073	-3.099	-1.190e-05	0.0003	0.302	0.272
sqr_000_06324	DyRh	2	-6.27	-6.774	2.500e-05	0.00069	0.357	0.222
sqr_000_06329	GeMn	2	-6.624	-6.636	-1.000e-06	0.00196	0.042	0.05
sqr_000_06331	EuTb	2	-2.969	-3.025	-8.000e-07	0.00142	0.189	0.135
sqr_000_06335	CoRu	2	-7.314	-7.944	0.000e+00	0.00087	0.369	0.429
sqr_000_06336	AlNi ₂ Yb	4	-4.098	-4.234	1.000e-06	0.00877	0.378	0.473
sqr_000_06337	TbTl	2	-3.725	-3.759	1.000e-07	0.00141	0.113	0.064
sqr_000_06339	NiPt	2	-5.317	-5.854	-1.000e-06	0.00575	0.238	0.382
sqr_000_06340	RhTb ₂ Zr	4	-5.506	-6.304	0.000e+00	0.00838	0.46	0.463
sqr_000_06345	CDy	2	-5.294	-6.839	-4.000e-06	0.00283	1.116	0.528
sqr_000_06347	CdTb	2	-2.442	-2.992	4.000e-07	0.00153	0.532	0.389
sqr_000_06348	AgPdUYb	4	-4.865	-5.149	6.000e-06	0.00491	0.914	0.263
sqr_000_06349	NbRu	2	-9.868	-9.919	1.000e-06	0.00219	0.164	0.128
sqr_000_06353	DySn	2	-4.599	-4.817	-1.040e-05	0.00341	0.469	0.255
sqr_000_06355	GdSi	2	-5.429	-5.507	0.000e+00	0.00158	0.47	0.34
sqr_000_06356	CoFe	2	-7.328	-7.459	-1.000e-06	0.00273	0.137	0.134
sqr_000_06358	CdDy	2	-2.716	-2.975	-4.030e-05	0.00509	0.333	0.173
sqr_000_06359	BiTb	2	-4.814	-4.918	-3.350e-05	0.00294	0.365	0.232
sqr_000_06362	InTb	2	-3.986	-4.043	3.000e-07	0.001	0.182	0.107
sqr_000_06365	MgRu	2	-4.993	-5.111	0.000e+00	0.00334	0.164	0.123
sqr_000_06372	AcSnYb	3	-2.979	-3.521	0.000e+00	0.00182	1.172	1.286
sqr_000_06373	PbYb	2	-3.048	-3.072	-8.000e-07	0.00438	0.257	0.194
sqr_000_06374	DyU	2	-6.671	-7.291	-2.700e-05	0.00264	0.887	1.065
sqr_000_06376	TbYb	2	-2.838	-2.853	3.000e-07	0.00034	0.094	0.086
sqr_000_06388	BeFe	2	-6.009	-6.028	-1.000e-06	0.00126	0.068	0.065
sqr_000_06389	GdZn	2	-3.191	-3.192	1.000e-07	0.00081	0.019	0.02
sqr_000_06390	RuSi	2	-7.812	-7.939	-1.800e-05	0.00678	0.114	0.073

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_06392	DyTb	2	-4.388	-4.519	-1.130e-05	0.00279	0.585	0.29
sqr_000_06394	InTb	2	-4.029	-4.043	-7.600e-06	0.00431	0.123	0.148
sqr_000_06398	GdZn	2	-3.189	-3.192	-2.800e-06	0.00202	0.029	0.039
sqr_000_06401	HgYb	2	-1.347	-1.483	-3.100e-06	0.00225	0.297	0.231
sqr_000_06402	MgNd	2	-3.214	-3.216	3.800e-06	0.00065	0.037	0.032
sqr_000_06403	BiYb	2	-3.405	-3.41	-1.900e-06	0.00129	0.053	0.014
sqr_000_06404	NdYb	2	-2.86	-2.994	-1.160e-04	0.00807	0.282	0.175
sqr_000_06407	DyHg	2	-2.663	-2.863	-1.000e-07	0.00125	0.27	0.122
sqr_000_06408	HgYb	2	-1.435	-1.476	-1.200e-06	0.0047	0.153	0.144
sqr_000_06409	Mn ₂ O ₂	4	-7.756	-7.835	-1.000e-06	0.0059	0.185	1.508
sqr_000_06413	TlYb	2	-2.189	-2.364	-2.000e-07	0.00136	0.353	0.277
sqr_000_06414	DyTe ₂	3	-4.427	-4.604	-4.000e-06	0.00295	0.84	1.091
sqr_000_06417	NdTl	2	-3.853	-3.867	7.900e-06	0.00481	0.321	0.23
sqr_000_06419	AlCo	2	-5.663	-5.985	-8.000e-06	0.00347	0.486	0.338
sqr_000_06421	Nd ₂	2	-4.259	-4.677	-3.400e-06	0.00684	0.388	0.475
sqr_000_06424	BeFe	2	-6.009	-6.028	-4.000e-06	0.00169	0.068	0.05
sqr_000_06428	DyZn	2	-3.17	-3.171	0.0000e+00	0.00062	0.04	0.026
sqr_000_06430	Be ₂ TbTi	4	-4.178	-4.807	-7.000e-06	0.00945	0.786	1.875
sqr_000_06431	Ni ₂	2	-5.158	-5.37	0.0000e+00	0.00429	0.185	0.082
sqr_000_06436	AuYb	2	-3.154	-3.321	-9.000e-07	0.00104	0.276	0.159
sqr_000_06438	FeRh	2	-7.266	-7.614	-4.000e-06	0.00259	0.423	0.395
sqr_000_06439	RuU	2	-10.141	-10.315	4.000e-06	0.00074	0.473	0.212
sqr_000_06442	GdZn	2	-2.996	-3.192	-1.000e-07	0.00316	0.29	0.189
sqr_000_06446	NiRu	2	-6.957	-7.184	3.000e-06	0.00381	0.321	0.352
sqr_000_06449	RhRu	2	-7.227	-8.11	-1.500e-05	0.00638	0.214	0.186
sqr_000_06450	MgRu	2	-5.099	-5.113	0.0000e+00	0.00513	0.08	0.058
sqr_000_06452	RuZn	2	-4.563	-5.003	-2.000e-06	0.00095	0.282	0.175
sqr_000_06457	CdDy	2	-2.685	-2.975	1.090e-05	0.00235	0.359	0.216
sqr_000_06458	CoV	2	-8.053	-8.153	-9.000e-06	0.00406	0.209	0.192
sqr_000_06459	AuYb	2	-3.142	-3.322	-7.000e-07	0.00402	0.29	0.177
sqr_000_06461	BiDy	2	-4.755	-4.878	-5.000e-07	0.00221	0.586	0.373
sqr_000_06463	RuY	2	-8.069	-8.089	1.000e-06	0.00366	0.082	0.054
sqr_000_06465	DyRh	2	-6.713	-6.767	3.000e-06	0.00647	0.115	0.094
sqr_000_06467	RhRu	2	-7.834	-8.176	-1.500e-05	0.00431	0.192	0.201
sqr_000_06468	CoFe	2	-7.363	-7.456	-1.000e-05	0.00544	0.181	0.156
sqr_000_06469	NiV	2	-7.142	-7.404	-2.000e-05	0.00257	0.189	0.341
sqr_000_06476	GaTb	2	-3.953	-4.33	-4.440e-05	0.00245	0.395	0.219
sqr_000_06479	GdYb	2	-2.791	-2.872	-3.510e-05	0.0024	0.21	0.13
sqr_000_06480	FeZn	2	-4.317	-4.321	-4.900e-06	0.00068	0.035	0.036
sqr_000_06483	RuTm	2	-6.96	-7.226	-3.700e-05	0.00391	0.186	0.1
sqr_000_06486	DySc	2	-5.211	-5.329	-5.600e-05	0.00357	0.33	0.455
sqr_000_06489	DyPd	2	-5.675	-5.764	0.0000e+00	0.00248	0.154	0.084
sqr_000_06490	NiRu	2	-7.028	-7.081	-7.000e-06	0.00716	0.092	0.078
sqr_000_06493	CRuSc ₂	4	-7.897	-8.087	0.0000e+00	0.00889	0.294	0.291
sqr_000_06495	AgNd	2	-3.959	-3.993	1.200e-06	0.00158	0.112	0.071
sqr_000_06496	FeRh	2	-7.285	-7.625	0.0000e+00	0.00448	0.233	0.177
sqr_000_06498	HgNd	2	-2.806	-2.917	2.600e-06	0.00482	0.179	0.117
sqr_000_06501	AlAsYb	3	-3.76	-3.852	-6.000e-06	0.00375	0.25	0.212
sqr_000_06502	CaYb	2	-1.447	-1.674	-8.700e-06	0.00064	0.491	0.831
sqr_000_06503	SbYb	2	-3.425	-3.593	-2.000e-07	0.00304	0.305	0.204
sqr_000_06504	Cu ₂ NdY	4	-4.817	-4.862	-5.000e-06	0.00271	0.368	1.744
sqr_000_06506	Co ₂	2	-6.815	-6.841	-2.900e-05	0.00748	0.075	0.058

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_06510	InTb	2	-3.965	-4.042	-1.500e-06	0.00214	0.149	0.091
sqr_000_06511	MgYb	2	-1.509	-1.526	-2.700e-06	0.00346	0.158	0.129
sqr_000_06516	DySbSi	3	-4.734	-5.067	1.000e-06	0.00422	0.464	0.51
sqr_000_06517	FeZn	2	-4.025	-4.327	-4.200e-06	0.0011	0.246	0.149
sqr_000_06518	CoDy	2	-5.546	-5.916	-9.000e-06	0.00349	0.337	0.233
sqr_000_06522	CoNi	2	-5.774	-6.07	1.000e-06	0.00442	0.356	0.52
sqr_000_06531	CoIr	2	-7.737	-7.88	-1.800e-05	0.00294	0.181	0.194
sqr_000_06533	Ni ₂	2	-5.302	-5.403	1.100e-05	0.00341	0.386	0.29
sqr_000_06535	Yb ₂	2	-1.286	-1.446	0.000e+00	0.00047	0.357	0.286
sqr_000_06539	RhTb	2	-6.697	-6.748	-1.800e-05	0.0082	0.108	0.06
sqr_000_06540	FeNi	2	-6.446	-6.639	-2.000e-06	0.00082	0.18	0.239
sqr_000_06542	CuNi	2	-4.421	-4.558	-3.460e-05	0.00992	0.232	0.221
sqr_000_06545	GaTb	2	-4.253	-4.324	3.000e-07	0.00113	0.195	0.184
sqr_000_06547	AlRu	2	-7.011	-7.138	-2.700e-05	0.00099	0.134	0.079
sqr_000_06549	DyU	2	-6.691	-7.319	-1.000e-06	0.00128	0.904	1.226
sqr_000_06550	NbNi	2	-7.569	-7.983	1.000e-06	0.00331	0.187	0.086
sqr_000_06551	DyRh	2	-6.718	-6.767	8.000e-06	0.00205	0.104	0.053
sqr_000_06552	CaYb	2	-1.418	-1.674	-7.730e-05	0.001	0.507	0.838
sqr_000_06555	CdNd	2	-2.961	-3.044	-1.800e-06	0.00237	0.163	0.106
sqr_000_06558	NdSn	2	-4.653	-4.951	-2.220e-05	0.00278	0.909	0.623
sqr_000_06563	AuTb	2	-4.744	-4.766	-8.900e-06	0.00619	0.085	0.056
sqr_000_06564	AlGd	2	-4.536	-4.564	3.000e-07	0.00129	0.108	0.066
sqr_000_06569	BiGd	2	-4.854	-5.014	-4.000e-06	0.00576	0.782	0.524
sqr_000_06575	RuV	2	-9.324	-9.339	-1.000e-06	0.00774	0.047	0.046
sqr_000_06579	AlCo ₃	4	-6.299	-6.338	-9.700e-05	0.0075	0.09	0.074
sqr_000_06580	DyP	2	-5.785	-6.582	0.000e+00	0.00302	1.264	0.861
sqr_000_06582	AsDy	2	-5.646	-5.727	-4.000e-06	0.00276	0.358	0.323
sqr_000_06585	CdYb	2	-1.367	-1.522	-1.500e-06	0.00505	0.348	0.305
sqr_000_06588	GdSe	2	-5.595	-5.6	0.000e+00	0.00193	0.056	0.066
sqr_000_06592	MgTb	2	-3.101	-3.12	-1.000e-06	0.00214	0.103	0.051
sqr_000_06594	Gd ₃ Pd	4	-4.13	-5.121	1.000e-06	0.00455	0.915	0.779
sqr_000_06595	MnNb	2	-8.972	-9.712	-1.000e-06	0.00073	0.55	0.274
sqr_000_06599	GdRh	2	-5.895	-6.731	6.000e-06	0.00263	0.515	0.303
sqr_000_06600	GdSc	2	-5.255	-5.359	-3.000e-06	0.00058	0.323	0.377
sqr_000_06601	AgTb	2	-3.96	-3.978	-1.600e-06	0.00451	0.077	0.066
sqr_000_06604	CoMn	2	-7.595	-7.932	-5.000e-06	0.00275	0.423	0.364
sqr_000_06606	CoIr	2	-7.519	-7.878	-1.800e-05	0.0028	0.172	0.103
sqr_000_06610	Ni ₂	2	-5.385	-5.415	-1.000e-06	0.00411	0.098	0.092
sqr_000_06612	Ni ₂	2	-5.088	-5.407	-1.000e-06	0.00562	0.225	0.25
sqr_000_06617	DyRu	2	-7.104	-7.179	-1.500e-05	0.00982	0.129	0.084
sqr_000_06618	RuV	2	-9.28	-9.33	3.000e-06	0.00159	0.14	0.105
sqr_000_06619	InYb	2	-2.515	-2.528	-1.500e-06	0.00244	0.08	0.045
sqr_000_06627	MgTb	2	-2.983	-3.119	-1.500e-06	0.0014	0.251	0.158
sqr_000_06630	MnTa	2	-10.402	-10.651	-1.190e-04	0.00246	0.149	0.118
sqr_000_06632	DyPt	2	-6.514	-6.53	-1.000e-05	0.00382	0.076	0.081
sqr_000_06633	CoRh	2	-6.783	-7.008	4.000e-06	0.00582	0.43	0.268
sqr_000_06634	GaGdGeZr	4	-5.236	-5.612	4.845e-03	0.00931	0.359	0.31
sqr_000_06639	GdZn	2	-3.085	-3.191	-9.900e-06	0.00505	0.207	0.159
sqr_000_06641	AgTb	2	-3.677	-3.985	-2.400e-06	0.00409	0.353	0.307
sqr_000_06644	PdTb	2	-5.75	-5.756	1.000e-06	0.00258	0.049	0.045
sqr_000_06646	CdNd	2	-2.485	-3.064	-8.300e-06	0.00235	0.585	0.347
sqr_000_06649	Ru ₂	2	-9.038	-9.131	-1.000e-06	0.00335	0.109	0.142

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_06652	NdSb	2	-5.203	-5.572	0.000e+00	0.00165	1.36	1.217
sqr_000_06654	GdMg ₂ Pd	4	-3.485	-3.58	-1.000e-06	0.00492	0.635	0.358
sqr_000_06664	GdYb	2	-2.837	-2.875	3.000e-07	0.00099	0.145	0.133
sqr_000_06667	DyPt ₃	4	-5.912	-6.714	-4.000e-06	0.00447	0.318	0.266
sqr_000_06676	GdTe	2	-5.085	-5.085	-1.000e-06	0.00322	0.019	0.016
sqr_000_06677	MnRu	2	-8.824	-8.98	-1.000e-06	0.00452	0.225	0.167
sqr_000_06681	GdLiSnTl	4	-2.587	-3.51	-3.000e-06	0.00494	1.159	0.784
sqr_000_06684	DyPt	2	-6.311	-6.532	0.000e+00	0.00139	0.22	0.126
sqr_000_06686	Fe ₂ SiZn	4	-5.824	-5.905	0.000e+00	0.00657	0.202	0.223
sqr_000_06687	DyZn	2	-3.163	-3.171	-3.500e-06	0.00146	0.061	0.049
sqr_000_06697	NdTl	2	-3.862	-3.868	-8.000e-07	0.00203	0.078	0.073
sqr_000_06698	NdTb	2	-4.274	-4.636	-2.400e-06	0.00201	0.536	0.641
sqr_000_06699	CdNd	2	-2.802	-3.061	-2.140e-05	0.00474	0.359	0.297
sqr_000_06702	MnRu	2	-8.834	-8.977	-2.300e-05	0.00714	0.177	0.171
sqr_000_06707	Cu ₂ GdHf	4	-5.032	-5.551	1.200e-05	0.00343	0.713	0.608
sqr_000_06711	NiOs	2	-8.025	-8.135	5.000e-06	0.00473	0.212	0.2
sqr_000_06719	InNd	2	-4.4	-3.649	-1.172e-02	0.00177	0.334	0.184
sqr_000_06725	GdTl	2	-3.413	-3.791	-5.760e-05	0.00174	0.43	0.244
sqr_000_06726	AuDyTl	3	-3.698	-3.78	-7.000e-06	0.00462	0.602	0.486
sqr_000_06727	AuMn	2	-5.451	-5.535	-1.100e-05	0.00396	0.458	0.232
sqr_000_06728	HgNd	2	-2.819	-2.931	-1.000e-06	0.00109	0.214	0.096
sqr_000_06736	YbZn	2	-1.521	-1.625	4.000e-06	0.00047	0.265	0.21
sqr_000_06738	Ga ₃ Nd	4	-2.869	-3.857	-8.000e-06	0.00556	0.525	0.448
sqr_000_06742	FeRu	2	-8.268	-8.549	0.000e+00	0.00229	0.147	0.19
sqr_000_06751	RuTb	2	-7.151	-7.155	-8.000e-06	0.00301	0.047	0.049
sqr_000_06754	AgDyGa	3	-3.694	-3.881	1.000e-06	0.00608	0.41	0.311
sqr_000_06758	CoFe	2	-6.945	-7.456	-4.000e-06	0.00352	0.502	0.353
sqr_000_06760	CeNd	2	-4.941	-5.183	-3.400e-05	0.00872	0.573	0.741
sqr_000_06762	CoFe	2	-7.347	-7.458	-9.600e-05	0.00312	0.144	0.082
sqr_000_06763	NiRu	2	-6.773	-7.191	-5.000e-06	0.00874	0.514	0.372
sqr_000_06764	Co ₂	2	-6.803	-6.838	0.000e+00	0.00331	0.104	0.098
sqr_000_06767	AuMn	2	-5.447	-5.546	-2.000e-06	0.00716	0.298	0.255
sqr_000_06768	MnRu	2	-8.549	-8.967	-2.400e-05	0.00506	0.183	0.308
sqr_000_06772	DyTl	2	-3.581	-3.73	-2.000e-05	0.00153	0.311	0.418
sqr_000_06775	AlNd	2	-4.565	-4.578	5.000e-07	0.00124	0.067	0.067
sqr_000_06778	MnNi	2	-7.082	-7.136	-1.000e-06	0.00337	0.079	0.049
sqr_000_06783	Mn ₂	2	-8.797	-8.912	1.000e-06	0.00472	0.255	0.224
sqr_000_06784	PtTb	2	-6.457	-6.523	0.000e+00	0.00387	0.116	0.078
sqr_000_06787	AcTb	2	-3.968	-4.262	-5.600e-06	0.00275	0.367	0.304
sqr_000_06788	SbYb	2	-3.127	-3.595	-1.300e-05	0.00449	0.545	0.276
sqr_000_06796	DyPd	2	-5.626	-5.757	-6.000e-06	0.00379	0.238	0.157
sqr_000_06797	RuZr	2	-9.495	-9.52	-8.000e-06	0.00368	0.085	0.056
sqr_000_06801	AlRu	2	-6.921	-7.117	-2.000e-06	0.00221	0.14	0.087
sqr_000_06802	CoMo	2	-8.589	-8.937	-2.300e-05	0.00184	0.4	0.479
sqr_000_06803	NdTl	2	-3.773	-3.863	-1.100e-06	0.0025	0.176	0.09
sqr_000_06806	DySb	2	-5.115	-5.447	0.000e+00	0.00049	1.437	0.996
sqr_000_06813	BeMn	2	-6.243	-6.321	0.000e+00	0.00046	0.106	0.088
sqr_000_06820	MnRh	2	-8.083	-8.093	0.000e+00	0.00091	0.032	0.032
sqr_000_06824	DyTl	2	-3.669	-3.724	-1.300e-06	0.00209	0.138	0.08
sqr_000_06828	NdS	2	-5.611	-6.15	-5.000e-06	0.00236	0.449	0.362
sqr_000_06829	GdYb	2	-2.866	-2.877	-2.000e-07	0.00071	0.08	0.037
sqr_000_06833	PrYb	2	-2.856	-3.015	1.800e-06	0.00083	0.304	0.201

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_06841	DyTe	2	-4.862	-4.995	-6.000e-07	0.00225	0.382	0.279
sqr_000_06842	CuNdTlZn	4	-2.561	-3.012	0.000e+00	0.00772	0.876	0.58
sqr_000_06846	IrNi	2	-6.999	-7.11	-3.000e-06	0.00353	0.301	0.202
sqr_000_06851	AsGd	2	-5.695	-6.143	0.000e+00	0.00026	1.34	1.173
sqr_000_06852	DyS	2	-5.906	-5.97	-1.300e-05	0.0028	0.128	0.1
sqr_000_06855	NiZr	2	-6.678	-7.346	-1.300e-05	0.00565	0.281	0.144
sqr_000_06856	Ru ₂	2	-8.513	-9.05	0.000e+00	0.00593	0.335	0.333
sqr_000_06858	GdRh	2	-6.635	-6.729	5.000e-06	0.00358	0.151	0.072
sqr_000_06862	HgNd	2	-2.879	-2.919	-2.000e-07	0.00079	0.113	0.055
sqr_000_06864	NiZn	2	-3.436	-3.538	-4.700e-06	0.00612	0.251	0.21
sqr_000_06870	NdTm	2	-4.541	-4.571	-1.700e-06	0.00156	0.181	0.302
sqr_000_06871	TlYb	2	-2.337	-2.341	5.000e-07	0.00201	0.051	0.035
sqr_000_06876	CoCu	2	-5.002	-5.05	-1.500e-05	0.00593	0.128	0.134
sqr_000_06879	GaRu	2	-6.322	-6.337	-6.000e-06	0.00478	0.067	0.041
sqr_000_06880	AsGd	2	-5.329	-6.165	0.000e+00	0.00464	1.289	0.859
sqr_000_06881	NaTb	2	-2.492	-2.501	-8.000e-07	0.00442	0.081	0.059
sqr_000_06884	CoMn	2	-7.839	-7.956	-1.000e-06	0.00163	0.135	0.096
sqr_000_06885	SnTb	2	-4.503	-4.847	-1.000e-07	0.00387	0.499	0.315
sqr_000_06891	NdRh ₃	4	-6.692	-6.825	-1.900e-05	0.00893	0.25	0.138
sqr_000_06893	MnRu	2	-8.402	-8.967	-5.000e-06	0.00408	0.297	0.367
sqr_000_06897	LiMn	2	-4.496	-4.964	0.000e+00	0.002	0.592	0.448
sqr_000_06898	DyTe	2	-4.548	-5.0	1.000e-07	0.00256	0.523	0.402
sqr_000_06902	Ni ₂	2	-5.223	-5.416	-4.000e-06	0.00619	0.352	0.557
sqr_000_06905	SiTb	2	-5.412	-5.499	-1.000e-06	0.00065	0.546	0.442
sqr_000_06906	NdY	2	-5.432	-5.551	-5.000e-06	0.00512	0.554	0.466
sqr_000_06910	GaTb	2	-3.944	-4.33	-2.660e-05	0.0024	0.405	0.212
sqr_000_06914	AgTb	2	-3.899	-3.978	-8.000e-07	0.00334	0.172	0.164
sqr_000_06915	CoIr	2	-7.672	-7.881	-1.400e-05	0.00393	0.248	0.117
sqr_000_06916	GdP	2	-6.09	-6.601	-9.000e-06	0.00201	1.215	1.092
sqr_000_06917	CeCo	2	12.046	-6.52	-3.200e-05	0.00734	1.135	0.895
sqr_000_06921	CdRu	2	-4.205	-4.386	-3.200e-06	0.00323	0.198	0.145
sqr_000_06922	AlFeNbNi	4	-6.568	-6.986	-2.700e-05	0.00639	0.668	0.713
sqr_000_06928	AgGd	2	-3.975	-3.984	-9.000e-07	0.00102	0.056	0.039
sqr_000_06931	MgNd	2	-3.121	-3.217	1.700e-06	0.00033	0.237	0.144
sqr_000_06932	GaMn	2	-5.777	-5.816	-2.000e-06	0.00397	0.081	0.098
sqr_000_06933	CuPdYbZn	4	-3.264	-3.269	0.000e+00	0.0067	0.076	0.041
sqr_000_06934	FeZr	2	-8.278	-8.583	-2.300e-05	0.00323	0.224	0.132
sqr_000_06936	CuDy	2	-4.159	-4.399	-1.753e-04	0.00305	0.297	0.196
sqr_000_06939	DyHg	2	-2.756	-2.849	-8.000e-07	0.00151	0.155	0.09
sqr_000_06940	DyTl	2	-3.694	-3.735	4.000e-07	0.00082	0.13	0.093
sqr_000_06942	AlDy	2	-4.528	-4.538	-1.800e-06	0.00249	0.06	0.042
sqr_000_06943	AlDyPd ₂	4	-5.046	-5.417	-3.000e-06	0.00389	0.337	0.338
sqr_000_06944	MgMn	2	-4.375	-4.686	-8.300e-06	0.00369	0.792	0.607
sqr_000_06945	AuGd	2	-4.589	-4.769	-1.000e-06	0.00243	0.249	0.153
sqr_000_06949	Ni ₂	2	-5.319	-5.408	-1.000e-05	0.00324	0.15	0.255
sqr_000_06951	Ru ₂	2	-8.87	-9.125	-1.000e-06	0.00385	0.248	0.278
sqr_000_06954	Co ₂	2	-6.747	-6.841	0.000e+00	0.00701	0.184	0.154
sqr_000_06957	DyGa ₂	3	-3.963	-4.087	-1.400e-05	0.00992	0.131	0.135
sqr_000_06971	RuSc	2	-7.987	-8.223	-2.300e-05	0.00129	0.182	0.107
sqr_000_06973	NiZn	2	-3.363	-3.535	-1.200e-06	0.00129	0.141	0.084
sqr_000_06975	RuV	2	-9.163	-9.322	1.000e-06	0.00824	0.135	0.075
sqr_000_06984	AgYb	2	-2.452	-2.525	3.600e-06	0.00154	0.218	0.212

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_06985	MnOs	2	-9.969	-10.02	-1.000e-06	0.00305	0.059	0.038
sqr_000_06987	NdSb	2	-5.045	-5.606	3.000e-06	0.00546	1.445	1.179
sqr_000_06988	AlCoCuDy	4	-4.703	-4.906	-2.000e-06	0.00392	0.555	0.467
sqr_000_06995	DyTe	2	-4.917	-4.992	-1.500e-05	0.00553	0.16	0.074
sqr_000_06998	AlDy	2	-4.531	-4.539	-3.000e-07	0.00235	0.057	0.042
sqr_000_07008	FePd	2	-6.02	-6.355	-3.000e-06	0.00843	0.423	0.344
sqr_000_07012	CoNd	2	-5.687	-5.793	1.200e-05	0.00886	0.183	0.113
sqr_000_07019	FeRh	2	-7.584	-7.614	-1.490e-04	0.00561	0.089	0.076
sqr_000_07021	GdMg	2	-3.1	-3.14	-1.700e-06	0.00124	0.175	0.096
sqr_000_07023	GdRh	2	-6.1	-6.728	5.000e-06	0.0001	0.417	0.238
sqr_000_07026	NdTl	2	-3.778	-3.877	-4.000e-06	0.00167	0.201	0.133
sqr_000_07028	MgNd	2	-3.214	-3.216	-1.800e-06	0.00159	0.033	0.029
sqr_000_07029	GdPd	2	-5.255	-5.737	-2.000e-05	0.00122	0.401	0.238
sqr_000_07030	ClGd	2	-4.103	-4.167	-2.000e-07	0.00179	0.172	0.111
sqr_000_07032	DyEr	2	-4.093	-4.439	-6.200e-06	0.00045	0.435	0.617
sqr_000_07034	TbZn	2	-2.94	-3.182	3.500e-06	0.00407	0.319	0.16
sqr_000_07037	TbTi	2	-5.806	-5.86	-2.200e-05	0.00495	0.136	0.254
sqr_000_07039	CoRh	2	-6.919	-7.014	-3.100e-05	0.00297	0.166	0.207
sqr_000_07045	CoDyPdZn	4	-4.753	-4.823	1.000e-06	0.00894	0.29	0.243
sqr_000_07046	DyMg	2	-3.07	-3.099	-2.000e-07	0.0003	0.252	0.147
sqr_000_07048	GdRu	2	-7.017	-7.141	-2.700e-05	0.00347	0.175	0.066
sqr_000_07051	BeCo	2	-5.652	-5.697	-2.100e-05	0.00517	0.099	0.06
sqr_000_07052	DyZr	2	-6.183	-6.36	-1.041e-03	0.00321	0.472	0.535
sqr_000_07053	CaGd	2	-2.925	-3.094	-3.200e-06	0.00539	0.389	0.562
sqr_000_07057	DySi	2	-5.396	-5.489	-3.000e-06	0.00152	0.55	0.608
sqr_000_07059	MgNd	2	-3.211	-3.216	6.000e-07	0.00055	0.058	0.05
sqr_000_07060	CoPt	2	-5.798	-6.482	-7.000e-06	0.00396	0.231	0.243
sqr_000_07061	NdSb	2	-5.036	-5.606	-5.000e-06	0.00221	1.439	1.148
sqr_000_07065	NiRu	2	-7.052	-7.193	-1.000e-06	0.00087	0.467	0.329
sqr_000_07067	RuTb	2	-7.031	-7.163	-1.000e-06	0.00279	0.168	0.1
sqr_000_07068	FeIr	2	-8.237	-8.532	-1.600e-05	0.00632	0.239	0.184
sqr_000_07070	Co ₂	2	-6.797	-6.839	-2.700e-05	0.00295	0.107	0.127
sqr_000_07080	TbTl	2	-3.666	-3.767	-2.400e-06	0.00113	0.198	0.121
sqr_000_07085	GdYb	2	-2.81	-2.873	-2.000e-07	0.00059	0.188	0.161
sqr_000_07086	NiPd	2	-5.255	-5.27	1.000e-06	0.00255	0.267	0.144
sqr_000_07087	CdTb	2	-2.929	-2.986	-1.060e-05	0.0022	0.145	0.088
sqr_000_07089	CoNi	2	-5.917	-6.061	-1.260e-04	0.00258	0.417	0.296
sqr_000_07093	GdSe	2	-5.556	-5.6	-1.000e-05	0.00461	0.116	0.109
sqr_000_07095	AlDyFeGa	4	-4.805	-4.937	-2.000e-06	0.00325	0.244	0.282
sqr_000_07097	ErTb	2	-4.021	-4.456	-3.200e-06	0.00168	0.376	0.309
sqr_000_07100	AgTb	2	-3.962	-3.979	-1.000e-06	0.00168	0.08	0.021
sqr_000_07109	Rh ₃ Tb	4	-6.024	-7.0	-2.100e-05	0.00743	0.337	1.066
sqr_000_07113	GdRh	2	-6.503	-6.723	-1.100e-05	0.00237	0.234	0.093
sqr_000_07115	CdYb	2	-1.33	-1.532	-2.360e-05	0.00191	0.402	0.35
sqr_000_07117	DyTl	2	-3.688	-3.732	-6.800e-06	0.00295	0.189	0.112
sqr_000_07120	SiTbU	3	-6.254	-6.915	-2.000e-06	0.00433	1.225	1.09
sqr_000_07123	CdGd	2	-2.975	-2.991	2.700e-06	0.00266	0.073	0.069
sqr_000_07124	FeNi	2	-6.51	-6.639	-4.000e-06	0.00528	0.132	0.046
sqr_000_07126	DyMg	2	-2.99	-3.098	2.500e-06	0.00274	0.207	0.145
sqr_000_07129	MnV	2	-9.238	-9.282	-1.000e-06	0.00191	0.122	0.07
sqr_000_07133	DyMg	2	-2.984	-3.098	-2.030e-05	0.00045	0.211	0.163
sqr_000_07134	CoMn	2	-7.814	-7.951	0.000e+00	0.00276	0.236	0.162

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_07136	Ru ₂	2	-8.473	-9.108	-1.000e-06	0.00814	0.47	0.301
sqr_000_07138	DyLi ₃	4	-2.302	-2.398	-1.340e-05	0.00571	0.837	0.438
sqr_000_07145	NdTb	2	-4.484	-4.627	-9.000e-07	0.00169	0.573	0.684
sqr_000_07147	DyYb	2	-2.767	-2.826	-6.000e-07	0.00203	0.176	0.082
sqr_000_07151	InYb	2	-2.505	-2.528	-1.600e-06	0.00295	0.111	0.086
sqr_000_07152	CoFe	2	-7.403	-7.459	-7.000e-06	0.00498	0.132	0.141
sqr_000_07153	DySb	2	-5.139	-5.456	-4.000e-06	0.00507	1.379	1.445
sqr_000_07159	InYb	2	-2.512	-2.528	-6.000e-07	0.00086	0.084	0.065
sqr_000_07160	AuCoNd	3	-4.694	-5.043	-3.100e-05	0.00876	0.565	0.366
sqr_000_07168	DySn	2	-4.734	-4.809	-2.500e-06	0.00122	0.38	0.276
sqr_000_07169	NdTl	2	-3.863	-3.869	1.100e-06	0.00086	0.065	0.061
sqr_000_07175	HDyPt	3	-5.298	-5.508	0.000e+00	0.00533	0.274	0.193
sqr_000_07178	GdMo	2	-7.05	-7.089	-3.000e-06	0.00189	0.104	0.071
sqr_000_07183	TbYb	2	-2.831	-2.852	-7.800e-06	0.00116	0.107	0.101
sqr_000_07185	TbTl	2	-3.516	-3.772	-9.100e-05	0.00155	0.332	0.302
sqr_000_07188	MgNd	2	-3.152	-3.215	-1.700e-06	0.00059	0.176	0.153
sqr_000_07191	YbZn	2	-1.519	-1.625	-5.200e-06	0.00033	0.267	0.195
sqr_000_07195	GdNd	2	-4.632	-4.642	5.000e-07	0.00114	0.079	0.1
sqr_000_07196	HgTb	2	-2.82	-2.862	4.000e-07	0.00122	0.108	0.084
sqr_000_07200	NdSb	2	-5.264	-5.573	-1.000e-06	0.00324	1.395	0.847
sqr_000_07201	DyNd	2	-4.317	-4.604	-2.000e-06	0.00466	0.436	0.623
sqr_000_07203	GdIn	2	-4.068	-4.071	-4.000e-07	0.00124	0.046	0.026
sqr_000_07212	RuTb	2	-7.129	-7.153	1.000e-06	0.00622	0.097	0.073
sqr_000_07215	CoMg	2	-3.99	-4.015	-1.140e-05	0.00224	0.121	0.074
sqr_000_07217	GdHg	2	-2.82	-2.874	-4.700e-06	0.0001	0.125	0.078
sqr_000_07222	BiGd	2	-4.587	-4.972	1.700e-06	0.00046	0.405	0.231
sqr_000_07224	SeYb	2	-4.125	-4.262	-3.520e-05	0.0039	0.238	0.17
sqr_000_07225	AgDy	2	-3.967	-3.972	-1.900e-06	0.00225	0.037	0.032
sqr_000_07226	AgNd	2	-3.99	-3.993	-2.000e-07	0.0009	0.043	0.034
sqr_000_07228	CoV	2	-7.985	-8.152	-2.000e-06	0.00243	0.373	0.256
sqr_000_07231	MoRu	2	-9.713	-9.966	2.000e-06	0.00264	0.3	0.352
sqr_000_07237	DyPd	2	-5.758	-5.762	-1.000e-06	0.00128	0.033	0.02
sqr_000_07241	GaGdNi ₂	4	-4.284	-4.926	-1.000e-06	0.00826	0.742	0.861
sqr_000_07243	GdSn	2	-4.745	-4.869	1.400e-06	0.00151	0.47	0.287
sqr_000_07246	IrRu	2	-8.513	-9.075	0.000e+00	0.00862	0.384	0.209
sqr_000_07249	ErNdSi	3	-4.322	-5.19	-9.000e-06	0.00639	0.335	0.687
sqr_000_07251	DyP	2	-6.02	-6.575	-1.000e-06	0.00321	1.315	0.928
sqr_000_07252	GdTl	2	-3.481	-3.79	-3.000e-07	0.00096	0.38	0.252
sqr_000_07253	DyMg	2	-3.039	-3.099	-2.800e-06	0.00081	0.185	0.097
sqr_000_07254	AgGd	2	-3.982	-3.984	-1.740e-05	0.00273	0.031	0.023
sqr_000_07256	GaYb	2	-2.621	-2.715	-3.390e-05	0.00061	0.243	0.15
sqr_000_07257	AgGd	2	-3.953	-3.985	8.000e-07	0.00125	0.15	0.089
sqr_000_07261	GdZn	2	-3.183	-3.192	-4.000e-07	0.00052	0.073	0.076
sqr_000_07263	DySc	2	-5.307	-5.31	-4.200e-05	0.00296	0.038	0.063
sqr_000_07265	GdSi ₂	3	-5.438	-5.694	-3.000e-06	0.00376	0.238	0.181
sqr_000_07267	DyPd	2	-5.748	-5.762	0.000e+00	0.00056	0.088	0.08
sqr_000_07269	AgDy	2	-3.803	-3.974	-1.900e-06	0.00364	0.252	0.159
sqr_000_07270	DyTl	2	-3.708	-3.733	-2.000e-07	0.0076	0.094	0.064
sqr_000_07272	AgNd	2	-3.974	-3.995	-7.000e-07	0.00176	0.096	0.076
sqr_000_07274	AsRu	2	-6.679	-6.952	-7.000e-06	0.00287	0.336	0.209
sqr_000_07275	RhTb	2	-6.688	-6.749	-6.000e-06	0.00054	0.116	0.085
sqr_000_07277	SYb	2	-4.376	-4.728	-1.600e-06	0.00379	0.386	0.28

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_07286	MnSc	2	-6.724	-7.281	7.000e-06	0.00712	0.528	0.463
sqr_000_07289	FeZn	2	-4.28	-4.345	-7.400e-06	0.00481	0.123	0.123
sqr_000_07296	TlYb	2	-2.093	-2.366	-8.500e-06	0.00236	0.465	0.258
sqr_000_07307	Hg ₂ Nd	3	-1.102	-2.084	5.000e-07	0.00316	0.526	1.777
sqr_000_07308	BeFeNiSi	4	-3.924	-6.155	0.000e+00	0.0066	0.457	0.423
sqr_000_07311	AlNd	2	-4.555	-4.581	1.700e-06	0.00152	0.115	0.108
sqr_000_07315	ErNd	2	-4.276	-4.596	-7.000e-07	0.0013	0.566	1.024
sqr_000_07319	FeZn	2	-4.292	-4.32	5.000e-07	0.00587	0.172	0.167
sqr_000_07320	RuZr	2	-8.655	-9.413	-1.300e-05	0.0019	0.641	0.456
sqr_000_07325	TbZr	2	-6.144	-6.358	2.000e-06	0.00034	0.448	0.621
sqr_000_07328	TbYb	2	-2.825	-2.852	1.700e-06	0.00322	0.124	0.118
sqr_000_07332	NiZn	2	-3.346	-3.54	8.000e-07	0.00316	0.223	0.099
sqr_000_07333	HgNd	2	-2.662	-2.94	-2.310e-05	0.00358	0.375	0.253
sqr_000_07334	Ag ₂ Gd	3	-3.538	-3.665	-3.000e-06	0.00187	0.166	0.138
sqr_000_07335	AgAuDySb	4	-3.247	-4.139	-1.000e-06	0.00431	0.447	0.479
sqr_000_07340	Yb ₂	2	-1.281	-1.446	-7.000e-07	0.0014	0.361	0.246
sqr_000_07345	AuMn	2	-5.396	-5.545	-2.100e-05	0.00276	0.317	0.433
sqr_000_07346	DyPr	2	-4.547	-4.616	-1.000e-07	0.00078	0.221	0.384
sqr_000_07348	AlGaNiRu	4	-5.839	-5.861	0.000e+00	0.00718	0.081	0.065
sqr_000_07352	CuNd	2	-4.355	-4.369	5.300e-06	0.0017	0.072	0.094
sqr_000_07357	AsDy	2	-5.65	-6.11	0.000e+00	8e-05	1.304	0.523
sqr_000_07358	GdZn	2	-2.938	-3.192	-2.000e-07	0.00148	0.333	0.183
sqr_000_07360	PdRu	2	-6.738	-6.953	-3.000e-06	0.00414	0.328	0.404
sqr_000_07362	CdNi	2	-2.256	-3.016	-2.100e-04	0.00393	0.285	0.137
sqr_000_07363	AgLiNdRu	4	-4.144	-4.519	-1.000e-06	0.0076	0.605	0.386
sqr_000_07366	GdNi ₃	4	-5.458	-5.46	-1.000e-06	0.00804	0.026	0.029
sqr_000_07369	Ru ₂	2	-8.472	-9.034	-1.000e-06	0.00796	0.335	0.247
sqr_000_07372	MnNi	2	-6.746	-7.135	-4.000e-06	0.00181	0.557	0.456
sqr_000_07375	CdDyIrPt	4	-5.326	-5.675	-4.000e-06	0.00706	0.286	0.289
sqr_000_07378	BeCo	2	-5.623	-5.696	-4.000e-06	0.00556	0.1	0.026
sqr_000_07381	MgTb	2	-3.088	-3.122	-5.100e-06	0.00012	0.134	0.124
sqr_000_07382	DyLu	2	-4.087	-4.419	0.000e+00	0.00665	0.361	0.517
sqr_000_07383	FePd ₂	3	-5.748	-6.0	-6.000e-06	0.00629	0.386	0.312
sqr_000_07387	NdTe	2	-4.985	-5.25	-2.000e-06	0.00325	0.435	0.341
sqr_000_07398	PdTb	2	-5.579	-5.753	-1.000e-06	0.00413	0.219	0.148
sqr_000_07400	MnRu	2	-8.527	-8.976	-2.000e-06	0.00832	0.313	0.326
sqr_000_07401	AgGdRh	3	-5.056	-5.242	1.300e-05	0.00652	0.249	0.314
sqr_000_07403	DyPSZr	4	-7.097	-7.19	4.000e-06	0.00386	0.321	0.198
sqr_000_07416	NdRh	2	-6.517	-6.6	-1.000e-06	0.00119	0.144	0.069
sqr_000_07419	MnZn	2	-4.612	-4.792	-1.650e-04	0.00729	0.491	0.285
sqr_000_07421	AgTb	2	-3.925	-3.982	-1.600e-06	0.0022	0.237	0.161
sqr_000_07427	AlCo	2	-5.782	-5.989	0.000e+00	0.00705	0.349	0.317
sqr_000_07428	ClGd	2	-4.134	-4.167	-2.800e-06	0.00277	0.126	0.084
sqr_000_07429	AlCo	2	-5.696	-5.984	-1.100e-05	0.00485	0.357	0.265
sqr_000_07430	AlYb	2	-2.745	-2.793	-5.000e-07	0.00042	0.16	0.108
sqr_000_07435	HgNd	2	-2.809	-2.917	-3.110e-05	0.00073	0.177	0.106
sqr_000_07438	HoMgPrYb	4	-2.968	-3.053	0.000e+00	0.00537	0.701	0.929
sqr_000_07439	NiSc	2	-5.692	-6.347	-2.000e-06	0.0069	0.781	0.839
sqr_000_07441	BeRuV ₂	4	-7.369	-7.885	0.000e+00	0.00315	0.277	0.928
sqr_000_07442	DyMg	2	-3.048	-3.098	4.000e-07	0.00123	0.147	0.133
sqr_000_07444	DyRh ₃	4	-6.061	-7.018	-4.300e-05	0.0032	0.335	0.274
sqr_000_07447	FeMn	2	-8.383	-8.525	-7.000e-06	0.0051	0.237	0.279

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_07448	CdGd	2	-2.98	-2.994	-8.200e-06	0.00587	0.09	0.089
sqr_000_07449	CdTb	2	-2.855	-2.987	4.000e-07	0.00139	0.24	0.151
sqr_000_07450	AlDy	2	-4.51	-4.538	-5.000e-07	0.00103	0.096	0.106
sqr_000_07452	GdSb ₃	4	-1.285	-4.656	-1.000e-05	0.00349	0.835	0.525
sqr_000_07454	FeZn	2	-4.232	-4.344	-1.380e-05	0.0028	0.227	0.19
sqr_000_07455	AsNd	2	-5.524	-6.191	-1.000e-06	0.00044	1.303	0.953
sqr_000_07459	GdTl	2	-3.747	-3.78	-7.100e-06	0.0032	0.244	0.181
sqr_000_07464	GdSe	2	-5.564	-5.6	-3.000e-06	0.00175	0.166	0.18
sqr_000_07470	DyPr	2	-3.953	-4.612	-1.400e-06	0.00219	0.528	0.76
sqr_000_07471	GdMg	2	-3.117	-3.14	2.100e-06	0.00119	0.111	0.094
sqr_000_07473	CoNi	2	-5.875	-6.062	1.000e-06	0.00331	0.435	0.405
sqr_000_07476	AsBeRu	3	-2.298	-5.58	-2.000e-06	0.00869	0.546	0.558
sqr_000_07478	CoPt	2	-6.151	-6.485	-4.100e-05	0.00649	0.185	0.103
sqr_000_07479	GdYb	2	-2.795	-2.872	7.000e-07	0.00078	0.209	0.108
sqr_000_07480	DyMg	2	-3.039	-3.099	4.000e-07	0.00044	0.167	0.072
sqr_000_07483	CoFe ₂ Si	4	-7.311	-7.34	-2.700e-05	0.00521	0.102	0.106
sqr_000_07485	DyMg	2	-3.051	-3.098	1.100e-06	0.00076	0.142	0.086
sqr_000_07489	IrRu	2	-9.01	-9.068	-4.000e-06	0.00134	0.093	0.1
sqr_000_07490	NdNiZn ₂	4	-2.937	-3.294	-2.000e-06	0.00665	0.931	0.924
sqr_000_07491	GdZn	2	-3.005	-3.192	-2.110e-05	0.0056	0.285	0.222
sqr_000_07492	MgYb	2	-1.516	-1.529	0.000e+00	0.00091	0.175	0.199
sqr_000_07496	PdRu	2	-6.728	-6.95	-1.000e-05	0.00181	0.31	0.414
sqr_000_07497	AlCo	2	-5.983	-5.989	-1.900e-05	0.00364	0.037	0.026
sqr_000_07499	Yb ₂	2	-1.363	-1.448	-1.098e-04	0.00593	0.28	0.164
sqr_000_07505	Ga ₂ MgTb	4	-2.77	-3.389	-1.000e-06	0.00607	0.724	0.585
sqr_000_07507	CoMn	2	-7.545	-7.946	0.000e+00	0.00345	0.407	0.285
sqr_000_07510	Yb ₂	2	-1.297	-1.447	2.000e-07	0.00224	0.346	0.209
sqr_000_07517	DyPt	2	-6.512	-6.53	-7.000e-06	0.00211	0.081	0.047
sqr_000_07518	GdS	2	-5.387	-6.038	1.000e-06	0.00107	0.476	0.29
sqr_000_07520	MnV	2	-9.175	-9.272	-7.800e-05	0.00572	0.108	0.08
sqr_000_07523	DyGaNi ₂	4	-4.192	-4.891	-1.000e-06	0.00655	0.495	0.431
sqr_000_07525	FePd	2	-6.305	-6.349	-2.000e-06	0.00183	0.12	0.156
sqr_000_07526	CoPt	2	-6.29	-6.491	-2.000e-06	0.00829	0.419	0.432
sqr_000_07529	DyS	2	-5.898	-5.97	-5.000e-06	0.00229	0.133	0.081
sqr_000_07534	GdNd	2	-4.458	-4.637	-5.000e-06	0.00275	0.347	0.554
sqr_000_07536	TbZn	2	-3.133	-3.183	-4.000e-07	0.00066	0.191	0.176
sqr_000_07538	DyZn	2	-3.165	-3.172	-7.200e-06	0.00171	0.067	0.057
sqr_000_07539	DyS	2	-5.904	-5.97	-1.000e-06	0.00196	0.156	0.155
sqr_000_07541	AsDy	2	-5.575	-6.12	0.000e+00	0.00189	1.129	1.163
sqr_000_07550	GdLi	2	-3.061	-3.093	-3.900e-06	0.00134	0.135	0.128
sqr_000_07552	GaNdPtSn	4	-4.54	-4.923	-3.500e-05	0.00746	0.832	0.673
sqr_000_07554	CoTb	2	-5.777	-5.907	-5.200e-05	0.00531	0.187	0.092
sqr_000_07555	DyP	2	-6.151	-6.255	-1.000e-06	0.00672	0.17	0.136
sqr_000_07557	MgTb	2	-3.083	-3.121	-5.800e-06	0.00413	0.203	0.136
sqr_000_07562	NdSr	2	-2.823	-2.968	1.200e-06	0.00149	0.367	0.387
sqr_000_07566	DyIn	2	-4.021	-4.023	-1.000e-07	0.00385	0.032	0.036
sqr_000_07567	TbTl	2	-3.756	-3.758	-5.000e-06	0.0009	0.033	0.011
sqr_000_07574	NdSe	2	-5.732	-5.737	0.000e+00	0.00049	0.052	0.057
sqr_000_07578	TbZn	2	-3.168	-3.183	-9.000e-06	0.00087	0.086	0.063
sqr_000_07581	GdIr ₃	4	-8.089	-8.135	-1.000e-06	0.00298	0.124	0.118
sqr_000_07583	MgRu	2	-4.785	-5.118	-2.000e-06	0.0027	0.287	0.151
sqr_000_07584	AgIr ₂ Yb	4	-5.471	-5.521	-8.000e-06	0.003	0.126	0.217

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_07588	GdRh	2	-6.17	-6.726	2.000e-06	0.00211	0.392	0.226
sqr_000_07596	FeRu	2	-8.545	-8.56	-2.000e-06	0.0045	0.062	0.055
sqr_000_07598	AsNdNi	3	-5.899	-5.978	-1.000e-06	0.00427	0.184	0.171
sqr_000_07603	AlMg ₂ Yb	4	-1.415	-2.083	-7.000e-07	0.00273	0.615	0.505
sqr_000_07607	DyHg	2	-2.776	-2.858	-3.320e-05	0.00036	0.166	0.11
sqr_000_07608	MgNd	2	-3.115	-3.22	5.000e-07	0.00403	0.208	0.123
sqr_000_07610	IrRh ₂ Yb	4	-6.407	-6.423	1.000e-06	0.00181	0.108	0.071
sqr_000_07615	NdP	2	-6.111	-6.59	-1.000e-06	0.00383	1.318	0.699
sqr_000_07617	DyHo	2	-4.209	-4.467	5.300e-06	0.00151	0.455	0.754
sqr_000_07619	As ₂ Gd ₂	4	-5.943	-6.175	-1.000e-06	0.00392	0.28	0.25
sqr_000_07622	HgYb	2	-1.368	-1.481	-7.200e-06	0.00152	0.268	0.121
sqr_000_07624	GaPtTbZr	4	-5.174	-6.235	-1.000e-06	0.00402	0.507	0.439
sqr_000_07626	GdTh	2	-5.917	-5.969	-9.000e-06	0.00374	0.181	0.239
sqr_000_07630	AuGd	2	-4.527	-4.77	-1.000e-07	0.00055	0.285	0.159
sqr_000_07632	DyMg	2	-3.036	-3.099	1.300e-06	0.00344	0.144	0.116
sqr_000_07635	RhRu	2	-7.679	-8.08	-8.000e-06	0.00266	0.382	0.191
sqr_000_07636	CoV	2	-8.109	-8.151	-7.000e-06	0.00279	0.145	0.177
sqr_000_07642	CoRu	2	-7.863	-7.952	-7.200e-05	0.00388	0.151	0.118
sqr_000_07644	FeLu	2	-5.07	-6.168	9.000e-06	0.0008	0.861	0.742
sqr_000_07646	CoRh	2	-6.599	-6.999	-1.300e-05	0.00811	0.182	0.118
sqr_000_07647	DyYb	2	-2.798	-2.828	-7.000e-07	0.00179	0.127	0.096
sqr_000_07650	DyZn	2	-3.155	-3.173	-1.280e-05	0.00483	0.096	0.048
sqr_000_07654	DyLi	2	-3.069	-3.072	-1.800e-06	0.00339	0.04	0.032
sqr_000_07657	AgYb	2	-2.453	-2.524	-2.200e-06	0.00149	0.263	0.176
sqr_000_07659	MgNd	2	-3.174	-3.22	-2.000e-07	0.0003	0.288	0.293
sqr_000_07660	BiTb	2	-4.838	-4.923	1.200e-06	0.00647	0.563	0.493
sqr_000_07661	AlTb ₂	3	-4.302	-4.538	-1.000e-06	0.00151	0.965	0.615
sqr_000_07664	CoNi	2	-5.85	-6.063	-1.000e-06	0.00177	0.413	0.279
sqr_000_07671	MnRh	2	-7.644	-8.083	-1.130e-04	0.00238	0.356	0.372
sqr_000_07673	GdPd	2	-5.695	-5.75	-1.200e-05	0.00445	0.209	0.081
sqr_000_07679	EuYb	2	-1.494	-1.656	4.000e-07	0.00022	0.378	0.204
sqr_000_07685	PtRu	2	-7.168	-7.529	1.000e-06	0.00102	0.356	0.399
sqr_000_07686	AlTb	2	-4.54	-4.55	-1.460e-05	0.00069	0.053	0.023
sqr_000_07687	RuZr	2	-9.511	-9.52	-3.000e-06	0.00065	0.032	0.018
sqr_000_07691	CoMn	2	-7.682	-7.961	0.000e+00	0.0019	0.376	0.394
sqr_000_07692	PdRu	2	-6.643	-6.943	-3.000e-06	0.00175	0.267	0.367
sqr_000_07696	FeIr	2	-8.436	-8.525	1.000e-06	0.00476	0.124	0.127
sqr_000_07699	AgGdMg	3	-3.006	-3.117	1.500e-06	0.00289	0.3	0.312
sqr_000_07706	TeYb	2	-3.359	-3.972	-8.000e-07	0.00154	1.413	1.373
sqr_000_07708	BiGd	2	-4.873	-4.956	-2.300e-06	0.00533	0.378	0.352
sqr_000_07713	GdPd	2	-5.643	-5.745	-1.500e-05	0.00193	0.243	0.173
sqr_000_07715	YbZn	2	-1.474	-1.625	1.860e-05	0.00158	0.335	0.214
sqr_000_07719	NdTl	2	-3.844	-3.867	-3.000e-06	0.00314	0.186	0.144
sqr_000_07720	CoNi	2	-5.906	-6.063	0.000e+00	0.00448	0.291	0.36
sqr_000_07722	RuV	2	-9.221	-9.33	-5.000e-06	0.00133	0.336	0.175
sqr_000_07726	CoNi	2	-5.993	-6.07	-5.300e-05	0.00207	0.137	0.129
sqr_000_07728	CoNi	2	-5.974	-6.074	-1.300e-05	0.00236	0.156	0.111
sqr_000_07734	HgNd	2	-2.572	-2.931	3.130e-05	0.00065	0.685	0.666
sqr_000_07735	PdTb	2	-5.723	-5.756	-1.000e-06	0.00149	0.176	0.198
sqr_000_07738	FeNi	2	-6.495	-6.638	-2.000e-06	0.00416	0.162	0.104
sqr_000_07739	NdSb	2	-5.133	-5.603	0.000e+00	0.00267	1.438	1.178
sqr_000_07740	MnNi	2	-6.985	-7.134	-3.000e-06	0.0036	0.27	0.194

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_07743	DyGa	2	-4.298	-4.302	-4.000e-07	0.00675	0.044	0.036
sqr_000_07746	DyTc	2	-7.174	-7.217	3.000e-06	0.00051	0.151	0.108
sqr_000_07747	DyHg	2	-2.76	-2.85	-4.000e-07	0.00063	0.169	0.179
sqr_000_07748	CoNd	2	-5.573	-5.79	-3.800e-05	0.00346	0.27	0.239
sqr_000_07750	CuNd	2	-4.206	-4.372	1.670e-05	0.00607	0.258	0.202
sqr_000_07751	PtRu	2	-6.923	-7.606	-1.900e-05	0.00916	0.425	0.365
sqr_000_07752	MgYb	2	-1.517	-1.529	1.000e-06	0.00227	0.169	0.165
sqr_000_07754	DyPd	2	-5.758	-5.762	-5.000e-06	0.00335	0.057	0.039
sqr_000_07755	FeTc	2	-8.901	-9.209	-1.000e-06	0.00511	0.265	0.183
sqr_000_07758	GdYb	2	-2.695	-2.867	-8.000e-07	0.00091	0.304	0.196
sqr_000_07759	CoV	2	-8.015	-8.158	-6.000e-06	0.00249	0.209	0.251
sqr_000_07765	AlMn	2	-6.234	-6.442	-3.000e-06	0.00149	0.19	0.145
sqr_000_07767	BeDy	2	-3.998	-4.045	3.600e-06	0.0025	0.144	0.09
sqr_000_07770	FeRu	2	-8.303	-8.553	-3.000e-06	0.00958	0.165	0.137
sqr_000_07771	RuZn	2	-4.902	-4.995	-2.400e-06	0.00231	0.148	0.12
sqr_000_07772	SeYb	2	-4.11	-4.262	-6.000e-07	0.00337	0.258	0.174
sqr_000_07774	RuZn	2	-4.67	-4.976	-7.000e-07	0.00221	0.297	0.184
sqr_000_07788	GdZn	2	-3.191	-3.192	-2.640e-05	0.0022	0.024	0.014
sqr_000_07789	GdGeLi	3	-4.182	-4.251	0.000e+00	0.00661	0.297	0.232
sqr_000_07799	RuSi	2	-7.813	-7.941	-1.300e-05	0.00099	0.156	0.138
sqr_000_07813	RuSm	2	-7.048	-7.06	-1.000e-06	0.00266	0.058	0.04
sqr_000_07815	RuTb	2	-7.135	-7.157	0.000e+00	0.00405	0.072	0.066
sqr_000_07816	GdHg	2	-2.814	-2.874	-1.800e-06	0.001	0.127	0.1
sqr_000_07817	InYb	2	-2.511	-2.527	-2.061e-04	0.00235	0.115	0.045
sqr_000_07820	HNiTb	3	-4.887	-4.909	-1.000e-06	0.00344	0.076	0.076
sqr_000_07821	CdDy	2	-2.961	-2.968	-2.000e-07	0.00249	0.069	0.049
sqr_000_07842	AsDy	2	-5.482	-6.131	-2.000e-06	0.00242	1.123	0.968
sqr_000_07844	HgNd	2	-2.862	-2.928	5.100e-06	0.00401	0.157	0.126
sqr_000_07845	GaGd	2	-3.955	-4.344	1.290e-05	0.00054	0.403	0.215
sqr_000_07852	RuTa	2	-10.715	-10.809	1.200e-05	0.00298	0.103	0.043
sqr_000_07854	AgDy	2	-3.811	-3.973	-4.200e-06	0.00168	0.278	0.308
sqr_000_07855	PdTb	2	-5.713	-5.757	1.000e-06	0.00527	0.122	0.085
sqr_000_07857	GdTl	2	-3.755	-3.781	-8.000e-07	0.00441	0.091	0.048
sqr_000_07858	AlNd	2	-4.564	-4.581	1.000e-06	0.00372	0.075	0.055
sqr_000_07863	RuTh	2	-8.016	-8.659	-2.600e-05	0.00367	0.581	0.646
sqr_000_07864	IrTb	2	-7.275	-7.513	-1.000e-06	0.00416	0.213	0.16
sqr_000_07865	DyPt	2	-6.513	-6.53	-1.000e-06	0.00117	0.059	0.043
sqr_000_07869	MnNi	2	-6.935	-7.145	-2.690e-04	0.00724	0.182	0.156
sqr_000_07871	AlGdHfPd	4	-6.223	-6.243	0.000e+00	0.00325	0.16	0.114
sqr_000_07872	GdRu	2	-7.026	-7.141	-3.000e-06	0.00107	0.163	0.13
sqr_000_07875	Dy ₂ MgSm	4	-3.732	-3.835	5.000e-06	0.00226	0.916	1.14
sqr_000_07879	GdY	2	-5.387	-5.492	-3.000e-06	0.00153	0.629	0.4
sqr_000_07882	LiTb	2	-3.083	-3.086	-4.000e-07	0.0031	0.045	0.027
sqr_000_07884	CdNd	2	-2.99	-3.044	1.700e-06	0.00512	0.139	0.123
sqr_000_07887	MnNi	2	-6.902	-7.145	-9.000e-06	0.00678	0.217	0.217
sqr_000_07889	Rh ₂ YbZn	4	-4.696	-4.768	-2.000e-06	0.00434	0.479	1.206
sqr_000_07890	BaYb	2	-1.163	-1.649	-4.300e-06	0.00201	0.722	0.304
sqr_000_07893	RuW	2	-10.772	-11.051	-1.000e-06	0.00437	0.277	0.237
sqr_000_07895	TbZn	2	-3.129	-3.183	-1.250e-05	0.005	0.145	0.088
sqr_000_07898	BeMnSi	3	-4.918	-6.191	-4.000e-06	0.00665	0.601	0.422
sqr_000_07899	YbZn	2	-1.532	-1.625	-7.820e-05	0.0027	0.253	0.103
sqr_000_07900	DyIn	2	-4.01	-4.021	-1.710e-05	0.00107	0.059	0.041

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_07905	AlAuVYb	4	-3.976	-4.364	-3.000e-06	0.00325	0.355	0.641
sqr_000_07907	TbZn	2	-3.178	-3.181	0.000e+00	0.00214	0.042	0.052
sqr_000_07913	AlDyMg ₂	4	-2.932	-3.032	-2.000e-06	0.0046	0.247	0.278
sqr_000_07918	FeRh	2	-7.314	-7.615	1.000e-06	0.00348	0.264	0.302
sqr_000_07921	GdTe	2	-5.002	-5.084	-3.000e-06	0.00438	0.194	0.109
sqr_000_07922	DyZn	2	-2.928	-3.172	2.300e-06	0.00151	0.318	0.22
sqr_000_07924	AgTb	2	-3.574	-3.987	-1.080e-05	0.00206	0.419	0.313
sqr_000_07925	Ni ₂	2	-5.161	-5.43	4.000e-06	0.00683	0.375	0.559
sqr_000_07928	FeNi	2	-6.42	-6.649	-1.000e-06	0.00264	0.371	0.521
sqr_000_07932	GdLiMg ₂	4	-2.079	-2.408	-3.900e-06	0.00348	0.845	0.431
sqr_000_07933	RuTc	2	-9.025	-9.757	0.000e+00	0.00459	0.524	0.237
sqr_000_07935	AlNi	2	-5.118	-5.268	-4.600e-05	0.00403	0.136	0.086
sqr_000_07938	MgNd	2	-3.18	-3.217	-4.000e-07	0.00211	0.153	0.147
sqr_000_07939	CoGd	2	-5.739	-5.891	-1.000e-06	0.00134	0.206	0.18
sqr_000_07941	AgGd	2	-3.978	-3.984	-1.200e-06	0.00069	0.057	0.029
sqr_000_07945	ScTb	2	-5.186	-5.341	3.000e-06	0.00202	0.28	0.491
sqr_000_07946	AgYb	2	-2.455	-2.525	-1.100e-06	0.00209	0.21	0.129
sqr_000_07949	SnYb	2	-2.86	-3.3	0.000e+00	0.0014	0.555	0.557
sqr_000_07955	GdSb	2	-5.04	-5.507	-1.400e-05	0.00397	1.406	1.13
sqr_000_07968	Mg ₃ Nd	4	-1.555	-2.425	4.000e-07	0.0018	0.98	0.501
sqr_000_07969	CoNi	2	-6.007	-6.071	-4.000e-06	0.00257	0.198	0.179
sqr_000_07970	CdDy	2	-2.709	-2.975	1.000e-07	0.00301	0.339	0.211
sqr_000_07975	CoNi	2	-5.92	-6.068	-1.500e-05	0.00041	0.18	0.244
sqr_000_07976	NiRh	2	-6.096	-6.316	0.000e+00	0.00206	0.44	0.338
sqr_000_07986	AgYb	2	-2.457	-2.525	-1.900e-06	0.00198	0.205	0.149
sqr_000_07990	AuNi	2	-3.87	-4.239	2.500e-06	0.0089	0.284	0.177
sqr_000_07993	BeCo	2	-5.635	-5.697	0.000e+00	0.00571	0.098	0.065
sqr_000_07996	AuNd	2	-4.709	-4.751	5.000e-07	0.00229	0.168	0.155
sqr_000_07999	TbZn	2	-3.151	-3.184	-4.900e-06	0.00365	0.11	0.069
sqr_000_08000	MgYb	2	-1.512	-1.526	-4.500e-06	0.00132	0.142	0.116
sqr_000_08002	RuZr	2	-8.739	-9.446	-3.000e-06	0.00251	0.57	0.59
sqr_000_08006	PrTb	2	-4.476	-4.636	-1.400e-06	0.00067	0.551	0.54
sqr_000_08007	LaYb	2	-2.886	-3.079	-2.000e-06	0.00035	0.352	0.224
sqr_000_08008	AlNd	2	-4.465	-4.583	2.000e-07	0.00141	0.215	0.109
sqr_000_08009	GdPt	2	-6.482	-6.51	-3.000e-06	0.00174	0.087	0.049
sqr_000_08010	NdRh	2	-6.579	-6.612	-1.000e-06	0.00666	0.087	0.064
sqr_000_08013	FeMo	2	-8.896	-9.389	-4.200e-05	0.00397	0.199	0.108
sqr_000_08015	SmYb	2	-2.845	-2.939	-1.900e-06	0.0005	0.23	0.105
sqr_000_08017	EuYb	2	-1.465	-1.654	-6.960e-05	0.00154	0.428	0.306
sqr_000_08018	CuNi ₂ Tb	4	-4.642	-4.994	9.000e-06	0.00702	0.311	0.262
sqr_000_08019	BeNi	2	-4.966	-5.085	-2.100e-05	0.00654	0.263	0.272
sqr_000_08023	MnTc	2	-9.433	-9.541	-1.570e-04	0.00941	0.391	0.265
sqr_000_08025	H ₂ Mn	3	-4.671	-4.864	-6.500e-05	0.00408	0.465	0.608
sqr_000_08027	PbYb	2	-2.813	-3.071	-1.170e-05	0.00635	0.424	0.183
sqr_000_08036	GdPt	2	-6.451	-6.511	0.000e+00	0.00069	0.125	0.03
sqr_000_08039	CrMn	2	-8.984	-9.182	-1.000e-06	0.00604	0.221	0.169
sqr_000_08045	SeTb	2	-5.558	-5.558	-5.500e-05	0.00326	0.013	0.009
sqr_000_08047	TeYb	2	-3.543	-3.816	-2.770e-05	0.00479	0.313	0.265
sqr_000_08050	LiNdRh ₂	4	-5.439	-5.532	0.000e+00	0.00185	0.166	0.177
sqr_000_08052	CoRh	2	-6.916	-7.019	1.900e-05	0.00121	0.176	0.122
sqr_000_08053	DyFeIrPt	4	-6.309	-7.196	3.000e-06	0.00584	0.347	1.063
sqr_000_08056	AuFe	2	-4.924	-5.121	-2.000e-06	0.00305	0.155	0.136

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_08058	DyGd	2	-4.159	-4.511	-2.000e-06	0.0022	0.361	0.734
sqr_000_08071	DySb	2	-5.042	-5.46	-6.000e-06	0.0029	1.368	1.153
sqr_000_08075	Rh ₃ Tb	4	-6.293	-7.02	0.000e+00	0.00172	0.301	0.191
sqr_000_08077	GdNd	2	-4.171	-4.643	-4.100e-06	0.00199	0.532	0.999
sqr_000_08081	NdZn	2	-2.987	-3.224	-8.180e-05	0.00251	0.336	0.199
sqr_000_08084	MgYb	2	-1.513	-1.526	-7.200e-06	0.00091	0.129	0.081
sqr_000_08085	Ni ₂	2	-5.311	-5.414	-4.600e-05	0.00539	0.404	0.467
sqr_000_08086	YbZr ₃	4	-5.735	-6.473	-1.000e-06	0.00183	0.504	0.333
sqr_000_08090	GdGe	2	-5.103	-5.253	0.000e+00	0.00104	0.572	0.445
sqr_000_08092	AuMn	2	-5.377	-5.538	0.000e+00	0.00258	0.21	0.133
sqr_000_08093	SnYb	2	-3.259	-3.346	-1.700e-06	0.00741	0.505	0.344
sqr_000_08096	AuTb	2	-4.485	-4.77	-3.900e-06	0.00282	0.295	0.18
sqr_000_08097	DySe	2	-4.934	-5.515	-2.000e-06	0.00494	0.532	0.431
sqr_000_08100	RuZr	2	-9.5	-9.53	-2.900e-05	0.0036	0.063	0.049
sqr_000_08101	TbY	2	-5.33	-5.474	0.000e+00	0.00557	0.559	0.458
sqr_000_08108	PtTb	2	-6.501	-6.521	-1.200e-05	0.00197	0.065	0.045
sqr_000_08109	MnNi	2	-6.771	-7.109	0.000e+00	0.00155	0.516	0.408
sqr_000_08111	Yb ₂	2	-1.362	-1.448	-1.300e-06	0.00202	0.3	0.183
sqr_000_08114	BeFe	2	-6.019	-6.028	-4.100e-05	0.00198	0.045	0.023
sqr_000_08115	CuDy	2	-4.292	-4.398	-5.500e-06	0.0002	0.185	0.084
sqr_000_08118	AgTb	2	-3.948	-3.978	-1.780e-05	0.0026	0.098	0.068
sqr_000_08121	MnPt	2	-7.304	-7.548	0.000e+00	0.00159	0.206	0.24
sqr_000_08122	Ru ₂	2	-8.465	-9.027	1.000e-06	0.00679	0.331	0.365
sqr_000_08124	AlGd	2	-4.557	-4.56	1.000e-07	0.00524	0.031	0.03
sqr_000_08125	NiZn	2	-3.496	-3.54	-1.200e-06	0.00139	0.218	0.227
sqr_000_08131	MgYb	2	-1.523	-1.526	-2.700e-06	0.00235	0.084	0.08
sqr_000_08139	CoSc	2	-6.683	-6.991	0.000e+00	0.00463	0.423	0.275
sqr_000_08141	AlYb	2	-2.653	-2.795	0.000e+00	0.00114	0.318	0.376
sqr_000_08142	HNi	2	-4.002	-4.44	4.000e-07	0.00423	0.71	1.221
sqr_000_08146	Ag ₂ Dy	3	-3.628	-3.667	0.000e+00	0.00233	0.178	0.142
sqr_000_08147	RuV	2	-9.223	-9.325	-3.000e-06	0.00918	0.097	0.08
sqr_000_08148	PrYb	2	-2.862	-3.015	6.700e-06	0.00187	0.298	0.22
sqr_000_08154	CdNd	2	-3.01	-3.045	-8.000e-07	0.00093	0.109	0.069
sqr_000_08156	GdTe	2	-5.066	-5.086	0.000e+00	0.0013	0.081	0.063
sqr_000_08157	TbYb	2	-2.766	-2.848	-2.000e-07	0.00245	0.216	0.105
sqr_000_08164	CoGdMnPd	4	-5.776	-6.261	-1.800e-05	0.00556	0.517	0.444
sqr_000_08172	AuNd	2	-4.734	-4.75	5.000e-07	0.00218	0.071	0.047
sqr_000_08176	GaNdTi ₂	4	-5.821	-5.917	-1.000e-06	0.00456	0.461	1.317
sqr_000_08179	NdTl	2	-3.724	-3.88	-1.900e-06	0.00165	0.258	0.145
sqr_000_08180	FePt	2	-6.796	-7.062	-1.000e-05	0.00539	0.276	0.28
sqr_000_08181	FeZn	2	-4.282	-4.324	-2.000e-07	0.00078	0.082	0.061
sqr_000_08185	AgNd	2	-3.964	-3.995	-4.300e-06	0.00074	0.108	0.073
sqr_000_08186	DyMg	2	-3.041	-3.101	-1.280e-05	0.00071	0.381	0.261
sqr_000_08187	NdRh	2	-6.441	-6.604	-1.100e-05	0.00662	0.205	0.137
sqr_000_08191	MnOs	2	-9.602	-10.011	-1.900e-05	0.00093	0.387	0.238
sqr_000_08195	AsNd	2	-5.676	-6.178	0.000e+00	0.00504	1.343	0.873
sqr_000_08196	NdSb	2	-5.306	-5.596	-9.000e-06	0.00782	1.38	1.432
sqr_000_08197	CdTb	2	-2.769	-2.988	-1.000e-07	0.00205	0.308	0.214
sqr_000_08199	GdTl	2	-3.596	-3.797	7.200e-06	0.00449	0.297	0.117
sqr_000_08202	Al ₂ PdTb	4	-3.649	-4.843	-1.000e-06	0.00939	0.547	0.592
sqr_000_08203	CMn	2	-8.239	-8.671	4.000e-06	0.00628	0.628	0.467
sqr_000_08204	PbYb	2	-3.052	-3.075	-1.100e-06	0.00148	0.194	0.173

Table S7. The profile of generated materials with Square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sqr_000_08208	RuTi	2	-8.926	-9.26	-4.100e-05	0.00487	0.3	0.195
sqr_000_08210	CoGdPSn	4	-5.345	-5.868	0.000e+00	0.00423	0.431	0.742
sqr_000_08213	FePd	2	-6.216	-6.349	-6.000e-05	0.006	0.227	0.193
sqr_000_08214	HgYb	2	-1.433	-1.476	-5.600e-06	0.00048	0.154	0.111
sqr_000_08215	MgTb	2	-3.019	-3.119	2.700e-06	0.00093	0.197	0.14
sqr_000_08216	DyRh	2	-6.711	-6.767	-3.100e-05	0.00834	0.114	0.05
sqr_000_08217	AgGd	2	-3.976	-3.984	-1.500e-06	0.00163	0.056	0.036
sqr_000_08220	PdYb	2	-3.896	-4.198	-1.150e-05	0.00139	0.376	0.3
sqr_000_08221	FeNi	2	-6.553	-6.632	-5.000e-06	0.00495	0.205	0.295
sqr_000_08223	NdTb	2	-4.452	-4.626	-4.000e-07	0.00054	0.56	0.752
sqr_000_08227	As ₂ HfYb	4	-5.098	-5.946	-5.000e-06	0.00483	1.177	1.552
sqr_000_08228	NdTl	2	-3.413	-3.877	-9.000e-07	0.00657	0.499	0.33
sqr_000_08229	PtTb	2	-6.501	-6.521	0.000e+00	0.0036	0.067	0.058
sqr_000_08230	FeNi	2	-6.444	-6.642	2.000e-06	0.00402	0.481	0.515
sqr_000_08231	GaYb	2	-2.623	-2.715	2.700e-06	0.00065	0.237	0.118
sqr_000_08232	DyTe	2	-4.45	-5.0	1.000e-07	0.00392	0.498	0.342
sqr_000_08233	DyRh	2	-6.713	-6.767	-2.000e-06	0.00336	0.107	0.069
sqr_000_08237	AgTb	2	-3.951	-3.978	-3.300e-06	0.00099	0.098	0.086
sqr_000_08240	GaNd	2	-4.357	-4.366	4.400e-06	0.0061	0.054	0.018
sqr_000_08243	CuDy	2	-4.379	-4.395	-1.100e-06	0.0034	0.071	0.05
sqr_000_08245	NiZn	2	-3.477	-3.541	-1.600e-06	0.00416	0.257	0.242
sqr_000_08246	GdRh	2	-6.565	-6.733	1.000e-06	0.00142	0.201	0.146
sqr_000_08247	Yb ₂	2	-1.312	-1.447	-1.800e-05	0.00275	0.33	0.272
sqr_000_08249	RuSc	2	-8.191	-8.253	-6.000e-06	0.00085	0.102	0.054
sqr_000_08252	MgTb	2	-3.093	-3.12	-2.200e-06	0.00127	0.108	0.044
sqr_000_08254	CdNd	2	-2.998	-3.046	2.000e-07	0.00195	0.127	0.057
sqr_000_08256	HfRu	2	-9.98	-10.363	-8.000e-06	0.00195	0.363	0.249
sqr_000_08260	SbYb	2	-3.589	-3.591	-3.000e-07	0.00102	0.06	0.044
sqr_000_08262	DyGa	2	-4.25	-4.305	-1.570e-05	0.00208	0.168	0.083
sqr_000_08263	DySc	2	-5.152	-5.323	1.000e-06	0.00083	0.296	0.399
sqr_000_08264	RuZn	2	-4.657	-4.971	-9.400e-06	0.00078	0.24	0.192
sqr_000_08266	FeNi	2	-6.431	-6.631	0.000e+00	0.00427	0.245	0.266
sqr_000_08267	CoRu	2	-7.395	-7.942	-1.000e-06	0.00647	0.376	0.391
sqr_000_08270	InYb	2	-2.516	-2.527	-1.001e-04	0.00422	0.068	0.064
sqr_000_08271	DyPd	2	-5.332	-5.748	-3.000e-06	0.00249	0.393	0.258
sqr_000_08280	MgNd	2	-3.214	-3.216	3.200e-06	0.0001	0.046	0.033
sqr_000_08282	CoV	2	-7.99	-8.156	6.000e-06	0.00119	0.264	0.179
sqr_000_08285	Mg ₃ Yb	4	-0.728	-1.493	4.000e-07	0.00472	0.703	0.669
sqr_000_08288	InTb	2	-3.85	-4.057	1.400e-06	0.00525	0.316	0.205
sqr_000_08289	DySc	2	-5.227	-5.298	-4.000e-06	0.00105	0.164	0.163
sqr_000_08290	NdPt	2	-6.243	-6.284	4.000e-06	0.00556	0.235	0.176
sqr_000_08293	DyGd	2	-4.106	-4.505	-1.670e-05	0.00131	0.371	0.557
sqr_000_08297	DySi	2	-5.397	-5.488	-3.000e-06	0.00264	0.557	0.428
sqr_000_08299	GdHg	2	-2.839	-2.873	6.000e-07	0.00142	0.097	0.057
sqr_000_08304	GdHo	2	-4.095	-4.49	-2.400e-06	0.00174	0.39	0.393
sqr_000_08305	SnYb	2	-2.841	-3.3	-2.000e-06	0.00407	0.57	0.377
sqr_000_08306	BiYb	2	-3.409	-3.41	2.400e-06	0.00096	0.05	0.039
sqr_000_08311	NdPd	2	-5.617	-5.694	-1.000e-05	0.00316	0.152	0.157
sqr_000_08315	FePd	2	-6.184	-6.344	-6.300e-05	0.00469	0.133	0.125
sqr_000_08317	GdGeHg	3	-3.049	-3.577	1.000e-06	0.00161	0.769	0.712
sqr_000_08320	DyEr	2	-4.353	-4.476	-4.800e-06	0.00208	0.567	0.301

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation

Index	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_00013	Ga ₂ Gd ₂ NiY ₂	7	-4.766	-5.157	-1.400e-05	0.00395	0.837	1.884
elt_000_00044	Ga ₃ Nd ₃	6	-3.966	-4.29	-2.000e-06	0.00463	0.785	0.768
elt_000_00110	As ₃ BaCdFe ₂	7	-4.548	-4.845	0.000e+00	0.00491	0.569	0.567
elt_000_00126	Dy ₃ Ga ₃	6	-3.812	-4.225	-1.000e-06	0.00502	1.161	1.513
elt_000_00136	Gd ₃ Sb ₂ V ₂	7	-5.842	-6.013	-3.000e-06	0.00491	0.382	1.393
elt_000_00148	BaCd ₂ Sb ₂ Yb ₂	7	-2.202	-2.649	-1.000e-05	0.00757	1.839	2.459
elt_000_00160	CoSe ₂ Tb ₂ Te	6	-5.157	-5.483	-3.140e-04	0.00835	0.801	0.975
elt_000_00171	Ga ₃ Gd ₃	6	-3.964	-4.254	-1.000e-06	0.00835	0.812	0.822
elt_000_00227	Dy ₂ MnPrSe ₂	6	-5.291	-5.69	1.000e-06	0.00604	0.373	0.731
elt_000_00250	BaGd ₂ Sn	4	-3.712	-3.887	-3.000e-06	0.00517	0.562	0.818
elt_000_00271	As ₄ Ru ₂	6	-6.055	-6.267	2.300e-05	0.0089	0.218	0.363
elt_000_00295	CdNd ₂ Te ₄	7	-3.76	-4.323	0.000e+00	0.00367	0.416	2.738
elt_000_00297	Sb ₂ Sr ₂ Yb ₂	6	-2.525	-3.329	2.000e-06	0.00549	1.768	1.854
elt_000_00308	Al ₄ SmYb ₂	7	-3.247	-3.402	0.000e+00	0.00317	0.806	0.981
elt_000_00324	CdGeSb ₂ Tb ₂ Te	7	-3.814	-4.224	-2.000e-06	0.00571	1.148	1.92
elt_000_00330	CaPdSb ₂ Tb ₂	6	-4.454	-4.985	-2.000e-06	0.00516	0.565	0.916
elt_000_00337	As ₃ Co ₂ Zn	6	-4.655	-4.88	-5.000e-06	0.00726	0.284	0.405
elt_000_00349	Ga ₃ Yb ₃	6	-2.374	-2.61	0.000e+00	0.00533	1.072	1.166
elt_000_00366	AgAs ₃ Dy ₂ Zn	7	-4.046	-4.488	0.000e+00	0.00633	1.059	1.316
elt_000_00392	Ni ₂ Sn ₄	6	-2.09	-4.38	-6.000e-06	0.00756	0.846	1.1
elt_000_00404	Al ₂ Gd ₃ Mg	6	-3.762	-4.059	0.000e+00	0.00328	1.207	2.696
elt_000_00410	CdNaSrTb ₂	5	-2.437	-2.516	-1.000e-06	0.00292	0.316	0.376
elt_000_00417	Gd ₃ GeRhSiV	7	-5.851	-6.091	-1.000e-06	0.00415	0.498	0.682
elt_000_00441	Sb ₂ Se ₂ Tb ₂ Zr ₂	8	-5.558	-6.172	0.000e+00	0.00358	0.515	0.667
elt_000_00464	AlGeMn ₂ NaSbTe	7	-4.394	-4.901	2.000e-06	0.00557	1.049	1.139
elt_000_00467	Cd ₃ CeRu ₂	6	-3.891	-4.395	-4.000e-06	0.00987	0.552	0.639
elt_000_00485	Sb ₄ Yb ₂	6	-3.457	-3.785	-1.000e-06	0.00467	1.211	1.199
elt_000_00525	Al ₂ CoFe ₂ Yb	6	-5.027	-5.34	-3.000e-06	0.00902	0.541	0.597
elt_000_00554	Gd ₃ MgPbSi	6	-4.161	-4.42	1.000e-06	0.00398	0.761	1.015
elt_000_00568	AsPtRu ₂ SnTe	6	-5.081	-5.925	3.000e-06	0.00626	0.597	0.701
elt_000_00608	Ga ₃ NaRu ₂	6	-4.123	-4.779	0.000e+00	0.00979	0.918	1.254
elt_000_00652	Ga ₂ ScTb ₃	6	-4.373	-4.617	-1.000e-06	0.00765	0.533	1.702
elt_000_00670	Cd ₂ Dy ₂ SbYb	6	-2.809	-3.048	0.000e+00	0.00598	0.592	2.229
elt_000_00683	Dy ₃ OsP ₂ Rh	7	-6.582	-7.049	2.000e-06	0.00263	1.086	1.209
elt_000_00709	GeNd ₃ Ni ₂ Se	7	-4.971	-5.367	-1.000e-06	0.00361	1.097	2.287
elt_000_00722	As ₃ ErMn ₂	6	-6.107	-6.391	7.000e-06	0.00699	0.726	0.646
elt_000_00727	Ga ₄ Tb ₄	8	-3.846	-4.206	-1.000e-06	0.006	0.839	1.239
elt_000_00748	LaNi ₂ SnTb ₂	6	-5.041	-5.289	-6.000e-06	0.00489	0.784	0.825
elt_000_00773	Dy ₃ MgPt ₂	6	-5.137	-5.288	1.000e-06	0.00687	0.416	0.609
elt_000_00774	Dy ₂ Sb ₂ SrTe	6	-4.212	-4.921	-1.000e-06	0.00508	1.011	1.496
elt_000_00794	EuTlYb ₂	4	-1.588	-1.982	-5.300e-06	0.00559	1.597	1.044
elt_000_00818	Gd ₂ Mn ₂ SiSr	6	-5.289	-5.727	1.100e-05	0.009	1.119	2.341
elt_000_00821	As ₂ FeLaNiTb ₂	7	-5.536	-6.05	-1.400e-05	0.00355	1.003	2.281
elt_000_00837	BaCdNd ₂ Zn	5	-2.577	-2.728	-3.700e-05	0.00402	0.74	1.003
elt_000_00847	Dy ₃ Ga ₃	6	-3.923	-4.23	-1.200e-05	0.00651	0.907	0.8
elt_000_00874	AgGa ₂ Gd ₃ MnPd	8	-4.673	-4.802	0.000e+00	0.00617	0.345	0.529
elt_000_00889	Au ₂ LaYb ₃	6	-3.153	-3.246	0.000e+00	0.00392	0.549	0.484
elt_000_00941	As ₂ Dy ₂ NiSbSi	7	-4.927	-5.452	-4.000e-05	0.00988	0.758	1.527
elt_000_00977	Cl ₂ NNd ₂ PTe	7	-4.96	-5.655	-1.000e-06	0.00856	1.061	0.917
elt_000_00979	Cd ₃ CoDy ₂ Mg ₂	8	-2.61	-2.798	-4.000e-05	0.00584	0.484	0.914
elt_000_00987	As ₂ CaCuDy ₂	6	-4.345	-4.783	1.000e-06	0.0064	0.923	1.522
elt_000_01028	Cu ₂ GaNd ₂ Sr	6	-3.497	-3.702	0.000e+00	0.00569	0.351	1.018

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_01044	AlGd ₂ Sb ₃	6	-4.313	-4.817	-1.000e-06	0.00455	1.25	1.58
elt_000_01054	NiSbSmSn ₂ Tb ₂	7	-4.691	-5.039	-1.000e-06	0.00604	0.988	1.529
elt_000_01055	Dy ₃ Ga ₃	6	-3.857	-4.228	0.000e+00	0.00663	0.832	0.996
elt_000_01056	As ₂ Br ₄ Ru ₂	8	-3.819	-4.432	0.000e+00	0.00437	0.534	1.783
elt_000_01058	CdGeK ₂ Yb ₂	7	-1.714	-1.896	1.000e-06	0.00626	1.04	1.403
elt_000_01074	AsCdPRu ₂ V	6	-5.94	-6.63	1.000e-06	0.00739	1.1	1.197
elt_000_01076	C ₂ Hf ₂ Mn ₂ Ti	7	-8.596	-9.14	-8.000e-06	0.00745	0.599	0.689
elt_000_01078	MnTb ₂ Te ₅	8	-4.713	-4.944	9.000e-06	0.00569	0.828	0.675
elt_000_01084	Dy ₃ GaPt ₂ Re	7	-6.309	-6.414	-3.000e-06	0.00604	0.389	0.502
elt_000_01098	Ga ₂ Nd ₃ Sn	6	-4.188	-4.52	-4.000e-06	0.00731	0.99	1.196
elt_000_01108	Al ₄ Gd ₂ Ti	7	-4.399	-4.885	-5.000e-06	0.00491	1.015	2.164
elt_000_01116	CeGa ₃ Gd ₂	6	-4.169	-4.415	-6.000e-06	0.00928	0.795	0.919
elt_000_01146	AuDy ₃ Pt ₂	6	-5.472	-5.911	-8.000e-06	0.00661	0.693	1.02
elt_000_01164	Al ₃ Nd ₂ Sm	6	-4.182	-4.534	-6.000e-06	0.0046	1.193	1.41
elt_000_01184	I ₄ Tb ₂	6	-3.566	-3.719	-8.000e-06	0.00343	0.821	0.961
elt_000_01201	Gd ₄ Se ₄	8	-5.555	-5.761	-3.000e-06	0.00405	0.731	1.497
elt_000_01204	Gd ₃ PdSrZn	6	-3.611	-3.89	0.000e+00	0.00194	0.764	1.964
elt_000_01211	As ₂ FeSrTeYb ₂	7	-3.787	-4.45	-1.000e-06	0.00644	1.101	1.491
elt_000_01235	Mn ₂ Sn ₄ V	7	-3.532	-5.658	-1.000e-06	0.0084	0.666	0.949
elt_000_01236	Gd ₂ IPtTe	5	-4.319	-5.035	0.000e+00	0.00682	1.035	4.035
elt_000_01258	AlGd ₃ Ge ₂	6	-4.687	-4.975	-1.000e-05	0.00786	0.66	0.896
elt_000_01288	Al ₂ Cu ₂ Y ₂ Yb ₂	8	-3.79	-4.086	-4.800e-05	0.00793	1.018	2.161
elt_000_01320	Ga ₃ Gd ₃	6	-3.959	-4.256	0.000e+00	0.00379	0.887	1.746
elt_000_01321	CoGa ₂ Nd ₃	6	-4.421	-4.866	1.000e-06	0.00221	1.87	2.093
elt_000_01336	As ₃ GeMn ₂ P	7	-5.367	-5.849	-5.000e-06	0.00678	0.625	1.82
elt_000_01344	AlCaCuDy ₂	5	-3.651	-3.757	-8.000e-06	0.00574	0.288	0.306
elt_000_01367	Gd ₃ Ni ₃ Tl	7	-4.698	-4.926	-1.000e-06	0.0082	0.893	1.368
elt_000_01374	AlGaPdSbTb ₂	6	-4.508	-4.895	-2.000e-06	0.00527	1.265	1.958
elt_000_01380	AlCdGaYb ₃	6	-2.014	-2.259	-1.100e-05	0.00576	1.736	3.041
elt_000_01402	Cr ₃ Dy ₂ ErSb ₂	8	-6.109	-6.278	-1.000e-06	0.0057	0.296	0.352
elt_000_01419	Co ₃ Ge ₃ Nd ₂	8	-5.454	-5.864	-9.000e-06	0.00879	0.944	1.914
elt_000_01428	CGdGeNd ₂ SbSn	7	-5.103	-5.648	0.000e+00	0.00667	1.614	3.019
elt_000_01433	Ga ₂ Gd ₂ NbPdWZn	8	-5.278	-5.817	1.000e-06	0.00757	1.103	1.989
elt_000_01443	GeMgNiSiTb ₃ Zn	8	-4.396	-4.482	-3.500e-05	0.00646	0.253	0.359
elt_000_01450	CoDy ₃ Ga ₃	7	-4.311	-4.73	-7.000e-06	0.00469	0.861	1.129
elt_000_01457	Cd ₄ Dy ₂ Sb	7	-2.156	-2.46	1.000e-06	0.00507	0.382	0.539
elt_000_01476	CoP ₂ Ru ₂ W ₂	7	-8.64	-9.013	0.000e+00	0.00796	0.467	0.981
elt_000_01497	Dy ₂ Ga ₄	6	-3.594	-3.874	-1.500e-05	0.00827	0.708	0.863
elt_000_01509	O ₃ SeTb ₄	8	-6.92	-7.047	0.000e+00	0.008	0.434	0.666
elt_000_01514	Nd ₃ PdSb ₂	6	-5.024	-5.441	-9.000e-06	0.00911	0.824	1.214
elt_000_01515	ISbTb ₂	4	-3.894	-4.555	-1.100e-05	0.00504	1.583	1.511
elt_000_01527	AlAuNi ₄	6	-4.702	-4.888	-2.000e-06	0.0087	0.195	0.261
elt_000_01539	Ga ₃ Nd ₃	6	-3.974	-4.29	-2.200e-05	0.00462	0.772	0.825
elt_000_01567	AcSbTb ₃ Y	6	-4.785	-5.021	0.000e+00	0.00244	0.835	0.792
elt_000_01580	As ₂ Ru ₂ Sc	5	-6.86	-7.097	1.000e-06	0.0078	0.355	1.516
elt_000_01607	Ge ₃ Tb ₃	6	-4.741	-5.278	0.000e+00	0.007	0.848	1.036
elt_000_01623	AlGd ₃ Pt	5	-5.127	-5.257	0.000e+00	0.00358	0.325	0.298
elt_000_01633	Dy ₃ Pt ₃ Sn	7	-5.847	-6.068	1.000e-06	0.00837	0.365	1.259
elt_000_01641	Ca ₂ Te ₄ Yb ₂	8	-3.698	-4.081	0.000e+00	0.00299	1.201	2.035
elt_000_01653	Mn ₂ Sb ₃ Sc	6	-5.361	-6.024	0.000e+00	0.00817	0.577	0.828
elt_000_01656	CdSbTb ₂ TeTm	6	-3.92	-4.375	-1.000e-05	0.00379	1.468	2.954
elt_000_01661	As ₄ CuNi ₂	7	-3.577	-4.736	-5.000e-06	0.00994	0.734	0.88

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_01665	HgPbTb ₂	4	-3.267	-3.701	-1.000e-06	0.00335	1.032	1.149
elt_000_01694	AuGa ₂ Gd ₂ Sr	6	-3.514	-3.758	-7.500e-05	0.00821	0.628	0.723
elt_000_01702	Co ₂ Ge ₃ Zr	6	-5.45	-6.205	1.000e-06	0.00496	0.926	0.897
elt_000_01764	Au ₅ MgTb ₂	8	-3.737	-3.99	-3.000e-06	0.00599	0.551	1.089
elt_000_01787	Dy ₂ OsSb	4	-5.812	-6.529	1.000e-06	0.00557	1.119	1.596
elt_000_01791	Sn ₂ Tb ₂	4	-4.032	-4.853	3.000e-06	0.00492	1.13	1.131
elt_000_01829	CrGd ₃ NiP ₂ W	8	-6.69	-6.923	3.000e-06	0.00715	0.358	0.44
elt_000_01830	Hg ₄ Nd ₂ Yb ₂	8	-1.777	-2.031	-3.000e-06	0.00275	0.488	0.849
elt_000_01838	P ₂ Ru ₂ Sn	5	-6.13	-6.862	-1.000e-06	0.00662	0.325	1.518
elt_000_01839	Hg ₃ Nd ₂ Pr	6	-2.643	-2.918	-7.000e-06	0.00729	1.247	2.434
elt_000_01858	Au ₂ CdNd ₃	6	-3.929	-4.113	-1.000e-06	0.00264	0.627	0.816
elt_000_01863	Ir ₂ SbSrYb ₃	7	-4.169	-4.469	0.000e+00	0.00517	0.728	0.902
elt_000_01865	GaRhSrTb ₂	5	-4.205	-4.595	-8.000e-06	0.00646	1.358	2.2
elt_000_01869	CdGd ₄ Ni ₂	7	-4.296	-4.513	2.000e-06	0.00413	1.137	1.419
elt_000_01886	Al ₃ Nd ₃ Sc	7	-4.487	-4.755	1.000e-06	0.00417	1.404	1.642
elt_000_01889	Gd ₂ Hg ₃ Y	6	-2.861	-3.051	-1.000e-06	0.00278	1.2	1.65
elt_000_01918	CeGa ₂ Nd ₂ Rh ₂	7	-5.376	-5.652	-2.000e-06	0.0076	0.872	0.69
elt_000_01932	Dy ₂ HoPPt ₂	6	-5.7	-6.404	-2.000e-06	0.00633	1.633	2.882
elt_000_01941	Al ₂ Ga ₂ Ru ₂	6	-5.281	-5.549	0.000e+00	0.00699	0.579	1.001
elt_000_01943	AlDy ₃ Ga ₂	6	-3.933	-4.35	1.000e-06	0.00784	1.0	1.998
elt_000_01944	CoPrTb ₂ Zn	5	-4.241	-4.451	-1.000e-06	0.00538	0.257	0.472
elt_000_01951	Ge ₃ Ru ₂ Y	6	-6.288	-6.677	-1.000e-06	0.00479	0.263	0.345
elt_000_01964	AuGeRu ₃ Si	6	-6.6	-6.819	-2.000e-06	0.0079	0.225	0.351
elt_000_01969	BFe ₂ GdRu ₂	6	-7.002	-7.602	0.000e+00	0.00693	0.8	1.006
elt_000_01972	P ₃ Tb ₂ Tl	6	-4.776	-5.244	-1.000e-06	0.00785	1.241	2.534
elt_000_01980	PrPtSb ₂ Tb ₂	6	-5.079	-5.592	0.000e+00	0.00629	1.05	2.468
elt_000_01992	Ga ₃ MgNd ₂	6	-3.48	-3.686	1.000e-06	0.00565	0.937	0.994
elt_000_02083	AuSb ₂ Tb ₄	7	-4.889	-5.003	-1.000e-06	0.00395	0.342	1.0
elt_000_02126	Tb ₃ Zn ₃	6	-2.818	-3.053	0.000e+00	0.00565	0.774	1.055
elt_000_02127	Dy ₃ Ir ₂ Si	6	-6.506	-6.895	0.000e+00	0.00427	0.887	1.937
elt_000_02136	As ₃ AuGd ₂ Pr ₂	8	-5.195	-5.374	-3.000e-06	0.00434	0.299	1.018
elt_000_02161	BaTb ₂ Te ₄	7	-4.511	-4.887	0.000e+00	0.00386	1.106	1.871
elt_000_02168	AgAu ₂ Dy ₂ Sr	6	-3.657	-3.868	-1.000e-06	0.00404	0.7	1.957
elt_000_02171	CdFe ₂ HoIrSi	6	-5.843	-5.962	-1.400e-05	0.00831	0.424	1.007
elt_000_02187	Al ₂ SrYb ₄	7	-2.019	-2.204	-1.000e-06	0.00288	0.529	0.593
elt_000_02209	Ga ₃ Nd ₂ ReSb	7	-4.789	-5.332	0.000e+00	0.00454	1.28	1.371
elt_000_02211	Cd ₂ Hg ₂ Tb ₂ Tl	7	-1.992	-2.061	0.000e+00	0.00292	0.378	0.53
elt_000_02254	As ₄ BMn ₂	7	-5.025	-6.115	-1.000e-06	0.00781	0.644	0.552
elt_000_02265	BaPbSbYb ₃	6	-2.557	-2.845	0.000e+00	0.0029	0.94	2.053
elt_000_02275	Dy ₂ SrZn ₄	7	-2.225	-2.346	-1.300e-05	0.00659	0.367	0.518
elt_000_02293	AlDy ₃ Ga	5	-4.066	-4.295	1.000e-06	0.00537	0.646	2.026
elt_000_02297	Co ₃ Dy ₃	6	-5.447	-5.845	9.000e-06	0.00535	0.907	1.208
elt_000_02314	Dy ₂ Te ₃ Zn	6	-3.76	-4.182	2.000e-06	0.00377	1.089	2.275
elt_000_02327	GeNd ₂ PtRb	5	-4.175	-4.537	-1.000e-06	0.00388	1.725	3.148
elt_000_02362	Ga ₃ LaNbTb ₂	7	-4.725	-5.021	-2.000e-06	0.0085	1.199	2.309
elt_000_02377	CdGe ₂ Nd ₃	6	-4.131	-4.45	0.000e+00	0.00434	1.135	1.187
elt_000_02402	CaDy ₂ Pd ₃	6	-4.85	-5.178	-3.000e-06	0.00819	0.752	0.926
elt_000_02427	As ₃ Gd ₂ TeV	7	-5.108	-5.695	0.000e+00	0.00794	1.523	1.706
elt_000_02438	CdDy ₃ Mg ₂	6	-2.677	-2.95	0.000e+00	0.00436	1.04	1.385
elt_000_02466	Ru ₂ Se ₄	6	-5.021	-5.579	-1.000e-06	0.00454	0.717	0.584
elt_000_02481	GeSn ₄ Tb ₂	7	-4.118	-4.531	-1.000e-06	0.00726	1.474	2.443
elt_000_02482	Dy ₆ Rh ₂	8	-5.458	-5.604	-1.000e-06	0.00721	0.637	0.725

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_02509	CoMoP ₂ Ru ₂	6	-7.811	-8.082	1.000e-06	0.00975	0.397	1.159
elt_000_02529	GaGe ₃ Nd ₂ Rb	7	-3.896	-4.0	-3.400e-05	0.0075	0.324	0.395
elt_000_02558	Au ₂ SbTb ₃	6	-4.428	-4.854	-3.000e-06	0.00507	0.646	1.013
elt_000_02560	Se ₂ Tb ₂ TiV	6	-5.336	-6.108	3.000e-06	0.00601	1.265	3.078
elt_000_02565	As ₃ MoRu ₂	6	-6.973	-7.216	0.000e+00	0.00897	0.326	0.249
elt_000_02578	CoGeNd ₄ Pd	7	-5.104	-5.463	1.000e-06	0.00796	0.78	0.852
elt_000_02603	As ₂ CeDy ₂ Pt	6	-5.606	-6.211	6.000e-06	0.00479	0.788	1.185
elt_000_02615	Dy ₃ Ga ₂ Sn	6	-4.091	-4.428	1.000e-06	0.00534	0.887	0.939
elt_000_02627	C ₂ EuGd ₂ Si ₂	7	-5.598	-5.91	-8.000e-06	0.00852	0.523	0.671
elt_000_02631	Cd ₂ Gd ₂ PbRb	6	-2.389	-2.629	2.000e-06	0.00333	0.964	1.091
elt_000_02636	Au ₄ CeTb ₂	7	-4.354	-4.61	1.000e-06	0.00446	0.694	0.804
elt_000_02651	Cl ₃ Dy ₂ NaP	7	-4.275	-4.602	-1.000e-06	0.00659	0.944	1.308
elt_000_02658	Dy ₃ PtSi ₂	6	-5.343	-5.861	0.000e+00	0.00593	1.275	1.619
elt_000_02679	Ca ₂ Ga ₂ SbYb ₂	7	-2.655	-2.876	-1.000e-05	0.00501	0.483	1.243
elt_000_02689	Dy ₂ Te ₃	5	-4.14	-4.998	-1.000e-06	0.00517	1.524	2.561
elt_000_02694	Ga ₃ Tb ₃	6	-3.855	-4.24	1.000e-06	0.00789	1.111	1.321
elt_000_02724	CoRhSe ₃ TiYb ₂	8	-4.878	-5.471	0.000e+00	0.0082	1.392	2.036
elt_000_02798	AsRu ₂ Te	4	-5.425	-6.446	-2.000e-06	0.01	0.729	1.904
elt_000_02807	CeGd ₃ PdSn ₂	7	-4.737	-5.076	-1.100e-05	0.00882	1.066	1.262
elt_000_02830	NbRhRu ₂ Sb ₃	7	-6.841	-7.118	-1.000e-06	0.00364	0.973	1.345
elt_000_02850	Al ₂ Bi ₂ IrTb ₃	8	-5.134	-5.207	-5.000e-05	0.00761	0.294	0.434
elt_000_02853	Fe ₄ Hf ₃ Sb	8	-7.979	-8.385	1.000e-06	0.00779	0.986	3.251
elt_000_02905	Dy ₂ MoP ₅	8	-5.924	-6.482	0.000e+00	0.00708	1.192	1.714
elt_000_02941	Au ₂ CoTb ₃	6	-4.582	-5.067	1.300e-05	0.00796	0.732	1.016
elt_000_02976	BaPdSn ₃ Yb ₂	7	-3.48	-3.728	-2.000e-06	0.00459	1.106	1.325
elt_000_02981	Ga ₂ GeTb ₃	6	-4.218	-4.499	-2.000e-06	0.0054	0.788	1.756
elt_000_02990	AlAu ₂ Nd ₄	7	-4.448	-4.599	-2.000e-06	0.00598	0.476	0.744
elt_000_03003	Ga ₃ Nd ₃	6	-4.015	-4.292	-5.000e-06	0.00425	0.902	0.897
elt_000_03059	HgPbYb ₂	4	-1.666	-2.297	-3.000e-07	0.00316	1.61	1.473
elt_000_03068	CaCd ₃ Yb ₂	6	-1.28	-1.477	1.000e-07	0.00561	1.082	1.199
elt_000_03097	Dy ₃ Zn ₃	6	-2.788	-3.045	0.000e+00	0.00391	1.133	2.44
elt_000_03156	As ₃ MoNi ₂	6	-4.203	-6.004	0.000e+00	0.00976	0.87	1.062
elt_000_03195	BrCl ₃ Gd ₂	6	-4.19	-4.521	-1.000e-06	0.00408	0.953	1.416
elt_000_03200	AsB ₂ Co ₂ Os	6	-6.731	-7.185	-2.100e-05	0.00868	0.415	0.438
elt_000_03204	Rh ₂ Sn ₂ Tb ₃ Tl	8	-5.117	-5.331	-1.000e-06	0.0046	0.421	0.498
elt_000_03238	EuGa ₃ Tb ₂	6	-3.466	-3.775	0.000e+00	0.00624	0.945	1.043
elt_000_03252	ErNiSnTa ₂ Tb ₂ Y	8	-6.535	-6.659	-1.000e-06	0.00488	0.377	0.462
elt_000_03306	Ga ₃ Gd ₃	6	-3.918	-4.254	-1.300e-05	0.0049	1.136	2.217
elt_000_03365	SnTb ₂ Y	4	-4.818	-5.176	-1.400e-05	0.00621	0.546	0.639
elt_000_03387	Fe ₂ Pt ₂ Ti ₂	6	-7.311	-7.857	-1.000e-06	0.00344	0.706	0.864
elt_000_03388	As ₂ Co ₂ CrNaSe ₂	8	-4.687	-5.247	-4.000e-06	0.00904	0.783	0.971
elt_000_03399	CdCo ₂ Nd ₃	6	-4.7	-4.801	-1.900e-05	0.00969	0.145	0.235
elt_000_03420	AlGaMn ₂ Zr ₂	6	-6.508	-7.003	-2.600e-05	0.00581	0.671	0.731
elt_000_03464	Dy ₄ Rh ₄	8	-6.567	-6.703	0.000e+00	0.0028	0.426	0.478
elt_000_03467	BHfPt ₂ Ru ₂ Si	7	-7.789	-8.012	5.000e-06	0.00656	0.731	1.742
elt_000_03482	CaGaNi ₂ Rh	5	-4.318	-4.818	-1.000e-06	0.00735	0.479	0.694
elt_000_03508	Fe ₃ LiSe ₂	6	-5.268	-5.677	-5.000e-06	0.00557	0.915	1.539
elt_000_03511	Se ₄ Tb ₂	6	-4.775	-5.426	-5.000e-06	0.0039	0.749	0.92
elt_000_03519	Dy ₂ PdSb	4	-4.811	-5.553	-6.000e-06	0.00376	1.641	1.788
elt_000_03529	AuGeMgRu ₂	5	-5.251	-5.529	0.000e+00	0.00426	0.298	0.502
elt_000_03534	Ca ₂ Nd ₂ SbSn ₂	7	-3.894	-4.168	0.000e+00	0.00265	0.696	1.308
elt_000_03539	GePt ₃ Ru ₂	6	-6.704	-6.881	-2.000e-06	0.0062	0.278	0.705

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_03554	LaTb ₂ Zn ₃	6	-2.922	-3.111	-2.000e-06	0.00556	1.039	0.973
elt_000_03563	Ga ₂ Nd ₃ Pd	6	-4.439	-4.773	-1.000e-06	0.00733	1.693	2.022
elt_000_03570	CeGaGe ₂ Nd ₂	6	-4.753	-5.093	-1.000e-06	0.00427	0.717	0.97
elt_000_03575	Ga ₃ Yb ₃	6	-2.374	-2.611	0.000e+00	0.00567	0.859	0.989
elt_000_03582	AlAs ₂ CoTb ₂ Y	7	-5.565	-5.875	-1.000e-05	0.00773	0.511	0.442
elt_000_03588	Cd ₂ Nd ₂ PtRbRh	7	-3.752	-3.924	-3.000e-06	0.00519	0.394	0.511
elt_000_03631	AuGaGd ₂ LaTl	6	-3.955	-4.176	-1.000e-06	0.00423	1.005	1.127
elt_000_03664	Ru ₂ Sn ₃ Ti	6	-5.259	-6.433	-4.000e-06	0.00787	1.124	1.065
elt_000_03693	GeMgNi ₃	5	-4.475	-4.686	2.000e-06	0.00776	0.585	0.711
elt_000_03695	GaGd ₃ Pt	5	-4.968	-5.109	-1.000e-06	0.00505	0.315	0.45
elt_000_03709	CoIrKSn ₃ Yb ₂	8	-3.948	-4.152	-1.500e-05	0.00641	0.877	1.323
elt_000_03716	AsLaMgSb ₂ SnYb ₂	8	-3.584	-4.011	0.000e+00	0.0071	1.06	1.161
elt_000_03732	Gd ₃ Ir ₂ SbSi	7	-6.175	-6.365	-1.900e-05	0.00547	0.287	1.413
elt_000_03733	Ga ₃ Nd ₃	6	-3.973	-4.292	-1.000e-06	0.00455	0.932	1.021
elt_000_03741	Al ₃ Tb ₃	6	-4.089	-4.495	-2.000e-06	0.00528	1.137	1.514
elt_000_03782	Ge ₂ Rh ₂ Tb ₄	8	-5.721	-5.912	0.000e+00	0.00671	0.839	0.848
elt_000_03787	Co ₂ Ga ₃ Y	6	-4.878	-5.073	-1.200e-05	0.00882	0.734	0.649
elt_000_03817	Dy ₂ Pt ₃ Sr	6	-5.384	-5.802	0.000e+00	0.00546	1.101	1.415
elt_000_03822	Ga ₃ Gd ₂ Sc	6	-4.161	-4.503	-3.000e-06	0.00555	1.114	1.274
elt_000_03827	Gd ₃ Ni ₂ Sb	6	-4.984	-5.37	0.000e+00	0.00709	1.013	2.049
elt_000_03859	Nd ₂ RuSeTe ₂	6	-4.942	-5.765	-1.000e-06	0.00328	1.087	1.728
elt_000_03860	Gd ₂ ILuTe ₃	7	-4.285	-4.821	-7.000e-06	0.00479	1.135	3.404
elt_000_03871	AgPrRuSn ₂ Yb ₂	7	-3.983	-4.266	-4.000e-06	0.00409	1.08	2.419
elt_000_03895	Al ₃ Dy ₃	6	-4.062	-4.481	-1.000e-06	0.00389	0.983	0.933
elt_000_03903	AsCdDy ₂ Ge ₂ SiTm	8	-4.622	-4.783	-4.000e-06	0.00621	0.383	0.506
elt_000_03909	CdGd ₃ SiSn	6	-4.067	-4.429	-1.000e-06	0.00786	1.187	1.764
elt_000_03923	GaRuTb ₃ Zn	6	-4.386	-4.838	-2.000e-06	0.00696	1.027	1.257
elt_000_03940	As ₂ Co ₂ GaN _a	6	-4.484	-4.691	-3.000e-06	0.00682	0.654	0.649
elt_000_03944	BaDy ₂ Si ₂ Te	6	-4.312	-4.756	-2.000e-06	0.00259	0.98	2.726
elt_000_03945	Sn ₄ Tb ₂	6	-4.195	-4.622	0.000e+00	0.00516	1.003	1.38
elt_000_03950	Cu ₂ EuGaTb ₂	6	-3.605	-3.856	1.000e-06	0.00925	0.988	0.939
elt_000_03954	CuDy ₃ Ga ₂	6	-3.908	-4.269	-3.000e-06	0.00636	1.81	2.068
elt_000_03962	Sb ₃ SrTb ₂	6	-4.169	-4.864	0.000e+00	0.00486	0.793	1.578
elt_000_03964	Ge ₂ HoRu ₂ Si	6	-6.415	-6.549	0.000e+00	0.0064	0.358	0.789
elt_000_03967	As ₂ Gd ₂ MgPr	6	-4.668	-4.969	-2.000e-06	0.00364	0.701	0.885
elt_000_03970	Os ₂ Yb ₅	7	-4.011	-4.26	-5.000e-06	0.0061	0.238	0.92
elt_000_03972	Dy ₃ Ni ₃ Pd	7	-5.104	-5.495	-5.200e-05	0.00784	1.151	1.313
elt_000_03975	AuRhRu ₂	4	-6.537	-6.89	1.000e-06	0.00491	0.783	0.373
elt_000_04009	Ag ₂ AlAs ₃ Yb ₂	8	-3.386	-3.806	-1.000e-06	0.00591	1.165	1.744
elt_000_04013	AgDy ₃ Ga ₂	6	-3.791	-4.099	0.000e+00	0.00598	0.85	1.097
elt_000_04021	AlCuNd ₄	6	-4.164	-4.469	3.000e-06	0.00603	0.819	1.825
elt_000_04052	Mn ₂ Zr ₄	6	-7.723	-8.591	-3.000e-06	0.00424	0.884	0.778
elt_000_04057	Al ₂ Nb ₄ Nd ₂	8	-6.743	-7.077	1.000e-06	0.00623	0.677	1.728
elt_000_04101	AlDy ₂ Sb ₄	7	-4.092	-4.702	2.000e-06	0.00917	1.376	2.27
elt_000_04118	CaGeMgTb ₂ TeTi ₂	8	-4.548	-4.78	-3.000e-06	0.00658	0.753	1.146
elt_000_04129	HgLaNd ₂	4	-3.54	-3.864	-1.000e-06	0.00503	1.07	0.915
elt_000_04130	Al ₃ NdTb ₂	6	-4.164	-4.513	0.000e+00	0.00135	1.078	2.176
elt_000_04180	CuNi ₂ Tb ₃	6	-4.67	-5.023	4.000e-06	0.00762	1.141	1.518
elt_000_04213	Al ₅ Gd ₂ Ti	8	-4.4	-4.522	0.000e+00	0.00433	0.542	0.981
elt_000_04237	Mo ₂ Ni ₃ Sn	6	-6.347	-6.86	-5.000e-06	0.00833	0.47	0.418
elt_000_04253	AsSb ₂ Yb ₃	6	-3.247	-3.761	-2.000e-06	0.00243	1.064	1.496
elt_000_04264	Dy ₃ Ga ₂ Ni	6	-4.224	-4.639	0.000e+00	0.00617	1.762	1.65

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_04271	Ga ₃ RhTb ₂	6	-4.444	-4.749	0.000e+00	0.00676	0.835	0.989
elt_000_04278	Dy ₂ Si ₃ SnTl	7	-4.46	-4.671	0.000e+00	0.00674	0.601	0.74
elt_000_04283	NiSn ₅ Yb ₂	8	-3.617	-3.724	0.000e+00	0.00304	0.28	0.505
elt_000_04303	Dy ₂ Pt ₂ SbY	6	-5.906	-6.393	-2.000e-06	0.00454	0.794	1.0
elt_000_04336	Au ₂ Dy ₃ Sn	6	-4.461	-4.654	0.000e+00	0.00421	0.781	1.87
elt_000_04352	EuPt ₂ Yb ₂ Zn	6	-3.549	-3.844	0.000e+00	0.0054	0.591	0.715
elt_000_04359	Ga ₂ Ni ₃ Sr ₂	7	-3.536	-3.95	1.000e-06	0.00884	0.983	1.339
elt_000_04361	Au ₃ NaRu ₂	6	-4.281	-4.579	1.000e-06	0.00609	0.703	0.964
elt_000_04406	As ₃ Ni ₃	6	-4.392	-5.174	-2.500e-05	0.00822	0.879	1.671
elt_000_04426	CeGd ₂ Si ₃	6	-5.343	-5.75	1.000e-06	0.00545	0.992	1.171
elt_000_04455	Dy ₃ Ga ₃	6	-3.855	-4.227	4.000e-06	0.00629	0.832	0.969
elt_000_04465	CdPt ₂ ScTb ₂	6	-5.238	-5.591	-1.300e-05	0.00712	1.095	1.982
elt_000_04469	CrDy ₂ PdS ₄	8	-5.92	-6.126	-4.000e-06	0.00639	0.36	0.391
elt_000_04488	GeNd ₂ Ni ₂ SrZn	7	-4.078	-4.229	-2.000e-06	0.00498	0.615	0.665
elt_000_04498	Hg ₃ LaNd ₂	6	-2.615	-2.835	1.000e-06	0.00315	0.656	0.866
elt_000_04510	MgNd ₂ Ni ₂ SnTb	7	-4.363	-4.49	-4.000e-06	0.00364	0.573	0.733
elt_000_04546	Gd ₂ Ni ₂ ScSe ₂	7	-5.166	-5.616	5.000e-06	0.00887	1.057	1.231
elt_000_04547	CeGe ₂ Ni ₃	6	-4.504	-5.482	-7.000e-06	0.00956	0.701	0.729
elt_000_04556	As ₃ Fe ₃	6	-5.583	-6.346	-4.100e-05	0.00912	0.85	1.852
elt_000_04558	AgCdDy ₃ Sn ₃	8	-3.954	-4.007	-4.000e-06	0.00664	0.594	0.61
elt_000_04559	Al ₄ Gd ₃	7	-4.224	-4.354	0.000e+00	0.00333	0.617	0.757
elt_000_04561	Cd ₂ Nd ₃ Sb	6	-3.572	-3.751	-4.000e-06	0.00521	1.0	1.045
elt_000_04567	CdGa ₂ Yb ₃	6	-2.021	-2.177	1.000e-06	0.00704	0.393	0.632
elt_000_04596	Mn ₃ Sb ₂ Tb ₃	8	-5.994	-6.254	-2.000e-06	0.00476	0.605	0.69
elt_000_04605	Dy ₂ GeSb ₂ Te ₂	7	-4.247	-4.647	-1.000e-06	0.00527	0.684	1.0
elt_000_04609	AcCsSb ₂ TlYb ₂	7	-2.866	-3.01	-5.000e-06	0.00581	0.365	0.471
elt_000_04622	Ga ₂ Nd ₃	5	-4.152	-4.323	-2.000e-06	0.00712	0.56	0.578
elt_000_04640	As ₂ GaNiRu ₂	6	-5.601	-6.078	-1.000e-06	0.00477	0.628	0.387
elt_000_04680	AgSn ₄ Tb ₂	7	-3.982	-4.328	2.000e-06	0.00392	1.082	3.166
elt_000_04701	As ₃ NiTb ₃	7	-5.331	-5.651	-5.000e-06	0.0068	0.707	0.786
elt_000_04721	Ge ₂ Nd ₃ NiSi	7	-5.043	-5.406	-4.000e-06	0.005	1.074	1.165
elt_000_04732	Ga ₂ GeMn ₂ Rh	6	-5.511	-5.951	-6.000e-06	0.00845	0.697	1.794
elt_000_04739	Co ₂ GeMn ₂ Pd	6	-6.724	-6.863	-1.000e-06	0.00604	0.269	0.376
elt_000_04750	Al ₂ GeNaTb ₂	6	-3.7	-4.007	-2.000e-06	0.00381	0.954	1.147
elt_000_04761	Cl ₄ Gd ₂	6	-4.365	-4.703	9.000e-06	0.00887	0.824	0.613
elt_000_04804	GaSn ₂ SrYb ₂	6	-2.804	-3.029	-1.000e-05	0.00559	1.495	1.556
elt_000_04806	Ga ₂ LiNd ₂ NiSr	7	-3.563	-3.771	-4.000e-06	0.00796	0.977	1.042
elt_000_04814	CoGd ₂ INiSi	6	-4.524	-5.167	-8.000e-06	0.00962	1.309	1.322
elt_000_04878	Co ₂ Nd ₃ Si	6	-5.514	-5.783	-9.900e-05	0.00769	0.75	1.795
elt_000_04920	AgBaGd ₂ GeTe ₂	7	-3.991	-4.327	0.000e+00	0.00357	0.171	1.726
elt_000_04922	SbSrTb ₂	4	-3.623	-4.152	-1.000e-06	0.00998	1.227	3.345
elt_000_04933	AsBeCo ₂ Ti	5	-5.911	-6.155	9.000e-06	0.00941	0.497	0.739
elt_000_04944	Br ₃ Nd ₂ S	6	-4.524	-4.796	0.000e+00	0.00437	1.163	1.153
elt_000_04945	As ₂ BNi ₂ W ₂	7	-6.8	-7.452	-1.800e-05	0.00929	0.684	0.888
elt_000_04955	Ge ₃ Tb ₃	6	-4.815	-5.173	-1.000e-06	0.00602	0.685	1.836
elt_000_04958	Ga ₂ MgTb ₃	6	-3.605	-3.909	0.000e+00	0.00417	0.905	0.923
elt_000_04968	AsBaGd ₂ Rh	5	-4.774	-5.274	-3.000e-06	0.00426	1.196	1.801
elt_000_05007	Ga ₂ Ni ₂ P ₂	6	-4.308	-4.742	-3.000e-06	0.00755	0.657	0.823
elt_000_05057	Si ₄ Tb ₃	7	-5.097	-5.781	-2.000e-06	0.00347	0.785	2.875
elt_000_05098	MgNi ₄ Sn ₂ W	8	-5.32	-5.508	-7.000e-06	0.00766	0.608	0.963
elt_000_05109	GaGeMn ₂ ScTa	6	-6.843	-7.396	-1.000e-06	0.00945	0.763	0.921
elt_000_05154	Fe ₂ PV ₂ Zr	6	-7.813	-8.214	-1.200e-05	0.00657	0.691	1.479

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_05178	Ga ₂ MgNd ₃ Pt	7	-4.068	-4.407	-1.000e-06	0.00341	0.793	1.527
elt_000_05192	Mn ₂ Se ₄	6	-5.001	-5.68	-2.000e-06	0.00624	1.368	1.074
elt_000_05193	Ga ₃ Nd ₂ Pr	6	-3.963	-4.292	-2.000e-06	0.00798	0.758	0.802
elt_000_05196	Si ₃ Tb ₂ Y	6	-5.414	-5.869	-2.200e-05	0.00499	0.801	1.079
elt_000_05237	CdGd ₂ ReSnTmZn	7	-4.263	-4.602	0.000e+00	0.00929	0.381	0.475
elt_000_05297	IrNd ₃ SiTl	6	-5.267	-5.664	-2.000e-06	0.0047	1.071	2.439
elt_000_05319	BaNd ₂ Sb ₃	6	-4.401	-4.965	-6.000e-06	0.00631	1.025	1.588
elt_000_05357	CdGa ₂ Nd ₃	6	-3.609	-3.835	0.000e+00	0.0066	0.871	0.946
elt_000_05378	PdSb ₃ Yb ₃	7	-3.669	-3.892	0.000e+00	0.00567	0.448	1.166
elt_000_05386	P ₂ PtRu ₂ VZr	7	-7.648	-8.027	-5.000e-06	0.00405	0.359	0.413
elt_000_05398	AuDy ₂ ReTe ₄	8	-4.921	-5.102	4.000e-06	0.00584	0.54	0.872
elt_000_05404	Yb ₃ Zn ₄	7	-1.429	-1.563	-1.000e-06	0.00304	1.101	1.426
elt_000_05405	Gd ₃ OsSi	5	-6.026	-6.415	0.000e+00	0.00276	0.6	2.467
elt_000_05406	Dy ₂ Zn ₅	7	-2.167	-2.435	-4.000e-06	0.00319	0.847	1.756
elt_000_05409	AsSi ₂ Tb ₃	6	-5.124	-5.712	-1.000e-06	0.00567	0.903	1.157
elt_000_05421	Ga ₃ SrYb ₂	6	-2.343	-2.594	-4.000e-06	0.00416	0.983	1.159
elt_000_05439	AlDy ₃ Ga	5	-4.077	-4.295	-2.000e-06	0.00531	0.675	0.699
elt_000_05446	Al ₆ Gd ₂	8	-3.784	-4.106	-3.400e-05	0.00296	0.471	0.299
elt_000_05462	CrNd ₂ SrTe ₃	7	-4.75	-4.897	-1.100e-05	0.00533	0.434	1.239
elt_000_05463	I ₂ Mn ₂	4	-3.137	-4.71	0.000e+00	0.00916	1.227	1.327
elt_000_05469	Au ₂ SbTmYb ₂	6	-3.476	-3.867	-9.000e-06	0.00772	0.823	1.029
elt_000_05471	Cu ₂ Gd ₃ Pt	6	-4.674	-5.057	-3.000e-06	0.00671	0.685	0.981
elt_000_05484	CdSb ₂ Yb ₂	5	-2.489	-3.13	-3.000e-06	0.00316	1.612	2.011
elt_000_05487	SbSrTb ₂	4	-3.653	-4.152	-1.700e-05	0.00754	1.103	1.845
elt_000_05494	AgFe ₂ Ge ₂ Na	6	-4.316	-4.741	-1.000e-06	0.00706	0.718	2.044
elt_000_05503	BaEuGd ₂	4	-2.886	-3.03	-6.000e-06	0.00389	1.023	1.31
elt_000_05505	Dy ₃ Ga ₂ Ru	6	-4.791	-5.219	0.000e+00	0.00689	1.62	2.492
elt_000_05507	Gd ₃ Ge ₂ Pt	6	-5.244	-5.596	0.000e+00	0.00375	0.927	0.897
elt_000_05523	HgISb ₂ Tb ₂	6	-3.366	-3.801	0.000e+00	0.00454	0.813	0.867
elt_000_05524	Co ₂ NiPrSb ₂	6	-5.257	-5.551	1.500e-05	0.00799	0.401	1.134
elt_000_05545	Cd ₄ Yb ₂	6	-1.104	-1.295	-6.000e-07	0.00442	1.509	1.922
elt_000_05556	Au ₂ MgSi ₂ Tb ₂	7	-4.275	-4.604	-4.000e-06	0.0052	0.666	0.784
elt_000_05572	Al ₄ Fe ₂	6	-5.182	-5.412	1.000e-06	0.00584	0.29	0.583
elt_000_05576	Ga ₂ Gd ₂ SbSr	6	-3.552	-3.956	-2.400e-05	0.00833	0.611	1.715
elt_000_05579	Al ₄ Tb ₂ Ti	7	-4.365	-4.852	-1.600e-05	0.00489	0.961	2.1
elt_000_05592	CdGaNd ₂ Sr	5	-2.96	-3.096	-3.000e-06	0.00483	0.427	0.6
elt_000_05597	CaPt ₃ Ru ₂	6	-6.087	-6.476	-4.000e-06	0.00713	0.414	0.235
elt_000_05664	Dy ₃ FeGa ₃	7	-4.385	-4.541	-1.000e-06	0.00448	0.295	0.383
elt_000_05666	Se ₃ Tb ₂ TiV	7	-5.758	-6.237	-3.000e-06	0.00619	1.004	1.789
elt_000_05667	Fe ₃ Si ₂ Tb ₃	8	-5.983	-6.359	-2.000e-06	0.00522	0.493	1.381
elt_000_05669	Gd ₃ Ge ₂ Pt	6	-5.143	-5.598	2.000e-06	0.00526	1.333	1.46
elt_000_05670	CoGeKNd ₃ PdSn	8	-4.417	-4.789	-1.100e-05	0.00796	0.712	1.203
elt_000_05673	CdDy ₂ Na	4	-2.622	-2.714	-5.000e-06	0.00397	0.472	1.876
elt_000_05675	Tb ₂ Te ₂	4	-4.409	-5.038	3.300e-05	0.00517	1.125	1.388
elt_000_05679	CeGaNd ₂ Rh ₂	6	-5.8	-6.0	-9.000e-06	0.00848	0.265	1.569
elt_000_05680	Gd ₂ SnSrTe ₂	6	-4.006	-4.537	0.000e+00	0.00345	0.9	1.343
elt_000_05682	Fe ₂ Mg ₄	6	-3.095	-3.49	-1.800e-05	0.00774	0.64	0.725
elt_000_05684	BaGd ₂ Pd ₂ Sb	6	-4.648	-4.911	-1.000e-06	0.00673	0.91	1.064
elt_000_05685	IrPtSiTb ₃	6	-6.131	-6.458	-1.000e-06	0.00444	1.194	1.911
elt_000_05690	As ₄ Fe ₂	6	-5.223	-5.838	-7.000e-06	0.00558	0.948	1.278
elt_000_05697	GeRu ₂ SbZr ₂	6	-6.358	-7.603	-3.000e-06	0.0067	0.462	0.596
elt_000_05700	Al ₃ Gd ₃	6	-4.14	-4.508	0.000e+00	0.00437	1.266	1.748

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_05710	As ₄ Dy ₂ Ti ₂	8	-5.772	-6.371	-1.000e-06	0.00789	0.804	1.218
elt_000_05717	I ₄ Nd ₂	6	-3.756	-3.848	2.000e-06	0.00538	0.397	0.409
elt_000_05724	Dy ₂ HoMnSbSi ₂	7	-5.572	-5.782	-5.000e-06	0.00722	0.629	0.832
elt_000_05731	As ₂ RuSiTb ₃	7	-5.9	-6.224	-1.000e-06	0.00486	0.699	0.912
elt_000_05747	Gd ₄ HgPb ₂ Rb	8	-3.119	-3.532	0.000e+00	0.00375	1.176	3.257
elt_000_05753	Ge ₂ Ni ₂ Zn ₂	6	-3.253	-3.838	-7.700e-05	0.00818	0.728	2.643
elt_000_05771	Dy ₂ RhTe ₂ Zr	6	-5.624	-5.856	0.000e+00	0.00466	0.359	0.603
elt_000_05781	Sn ₅ Yb ₂	7	-3.328	-3.555	-6.000e-06	0.00517	1.191	1.976
elt_000_05782	AuCd ₂ Gd ₂ SbSrZn	8	-2.734	-3.013	-2.000e-06	0.00457	0.782	1.089
elt_000_05801	Dy ₃ PtSi ₂	6	-5.459	-5.86	0.000e+00	0.00343	0.787	0.87
elt_000_05834	Sn ₃ Yb ₃	6	-2.967	-3.194	-1.000e-06	0.00589	0.902	1.017
elt_000_05837	PrSbSi ₂ Tb ₂	6	-5.032	-5.524	-1.500e-05	0.00537	0.803	1.171
elt_000_05841	Ge ₃ NdRu ₂	6	-6.127	-6.387	-1.000e-06	0.00534	0.616	0.858
elt_000_05857	Ga ₂ Gd ₂ SbSr	6	-3.602	-3.954	-8.000e-06	0.00708	0.919	1.204
elt_000_05864	NdPtRu ₂	4	-6.994	-7.226	-1.000e-06	0.00767	0.646	0.294
elt_000_05868	Dy ₅ Ni ₂	7	-4.835	-4.993	-6.000e-06	0.00428	0.195	0.363
elt_000_05879	AsDy ₂ GaTe	5	-4.241	-4.794	-2.000e-06	0.00393	1.087	2.218
elt_000_05886	Al ₂ CoGeSbTb ₂	7	-4.732	-5.162	0.000e+00	0.00832	0.821	0.943
elt_000_05898	AsMn ₂ PSn ₂	6	-5.211	-5.868	3.000e-06	0.00477	0.519	0.828
elt_000_05968	Dy ₂ LaSb ₃	6	-4.824	-5.335	-6.000e-06	0.00584	0.85	1.221
elt_000_05976	SbSn ₃ Tb ₂	6	-4.249	-4.699	-1.000e-06	0.00829	0.892	0.954
elt_000_05977	AlGd ₂ InTe ₂ Tl	7	-3.968	-3.918	-1.000e-06	0.00359	0.683	0.658
elt_000_05990	C ₂ FeMn ₂ Nd	6	-7.596	-8.039	-1.000e-06	0.00856	0.595	1.088
elt_000_05995	GaGd ₂ IrRhSn ₃	8	-5.063	-5.404	-2.000e-06	0.00349	0.504	0.706
elt_000_06006	Ru ₂ Se ₄	6	-5.032	-5.539	1.000e-06	0.00579	0.614	0.934
elt_000_06024	Dy ₂ SbSiSnYb	6	-4.202	-4.599	-7.000e-06	0.00771	0.641	0.903
elt_000_06054	AlMgNd ₂ NiSr	6	-3.548	-3.727	-4.000e-06	0.00435	0.501	0.365
elt_000_06060	CBHfMn ₂ S ₃	8	-6.104	-7.352	-4.000e-06	0.00599	1.017	1.503
elt_000_06080	AgGa ₂ NaRu ₂	6	-4.361	-4.649	-3.000e-06	0.00645	0.609	1.253
elt_000_06090	Cd ₃ Dy ₂ Rb	6	-1.75	-2.051	-7.000e-06	0.00369	0.99	1.188
elt_000_06096	AsHfMnNi ₂ Si	6	-6.29	-6.826	1.800e-05	0.00937	0.552	0.708
elt_000_06114	Al ₂ Ru ₂ Si ₂	6	-6.202	-6.488	-8.000e-06	0.00729	0.431	0.765
elt_000_06124	CuFe ₂ Pt	4	-6.124	-6.347	-1.800e-05	0.0078	0.257	1.322
elt_000_06125	CdTb ₃	4	-3.425	-3.762	-3.000e-06	0.00443	0.789	1.96
elt_000_06150	AsDy ₃ Ir ₂ V	7	-6.551	-6.865	-5.000e-06	0.00549	0.925	1.254
elt_000_06154	RhSbSnTe ₂ Yb ₂	7	-3.578	-4.09	-1.000e-06	0.00325	1.176	1.354
elt_000_06160	Al ₂ Ga ₂ Ni ₂ Tb ₂	8	-4.204	-4.504	0.000e+00	0.00457	0.976	2.146
elt_000_06161	Al ₃ AuYb ₄	8	-2.552	-2.919	-2.000e-06	0.00607	1.535	2.261
elt_000_06190	Gd ₃ NNiSe ₃	8	-5.695	-6.215	-5.000e-06	0.00623	1.382	2.078
elt_000_06219	Al ₂ Gd ₂ GeYb	6	-3.776	-4.1	-1.000e-06	0.00494	0.976	1.118
elt_000_06245	Dy ₆ NbNi	8	-5.032	-5.278	3.000e-06	0.00736	0.39	1.833
elt_000_06247	Nd ₂ Sb ₃ Sr	6	-4.192	-4.951	0.000e+00	0.00303	1.223	1.774
elt_000_06271	CdGaGeSrTb ₂	6	-3.173	-3.472	0.000e+00	0.00885	1.26	2.449
elt_000_06309	GaGd ₂ LaPt	5	-4.98	-5.181	-3.000e-06	0.00935	0.593	0.678
elt_000_06330	Al ₃ Dy ₃ Zn	7	-3.53	-3.972	0.000e+00	0.00448	0.966	2.334
elt_000_06335	BaGd ₂ MgPd	5	-3.66	-3.758	-2.000e-06	0.00353	0.486	0.699
elt_000_06349	As ₃ MoRu ₂	6	-6.557	-7.199	1.000e-06	0.00671	0.424	0.414
elt_000_06418	As ₃ Co ₂ Zn	6	-3.984	-4.917	-7.000e-06	0.00727	0.6	1.096
elt_000_06423	Dy ₃ PtSi ₂	6	-5.46	-5.888	-1.400e-05	0.00328	1.239	1.771
elt_000_06439	CaSrYb ₂ Zn ₂	6	-1.469	-1.613	-5.400e-06	0.00338	0.332	0.436
elt_000_06444	Pd ₃ Tb ₃	6	-5.277	-5.701	-3.900e-05	0.00792	0.658	1.011
elt_000_06445	Sn ₄ Yb ₂	6	-3.249	-3.529	-5.000e-06	0.00835	1.1	1.103

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_06476	Dy ₃ MgSr ₂	6	-2.785	-2.92	-1.000e-05	0.00375	0.65	0.48
elt_000_06490	AgGd ₂ Ge ₂ Sr	6	-3.884	-4.19	-2.000e-06	0.00492	1.054	1.417
elt_000_06491	Au ₂ Nd ₃ Si	6	-4.665	-4.938	2.000e-06	0.00363	1.268	1.67
elt_000_06494	LaTb ₂ Zn ₄	7	-2.676	-2.855	-1.400e-05	0.00427	0.827	1.752
elt_000_06504	AlCuGaRu ₂ Sm	6	-5.432	-5.7	-1.100e-05	0.00766	0.491	0.408
elt_000_06507	CoEuGd ₂ GeLaRh	7	-5.232	-5.425	-7.000e-06	0.00868	0.815	0.955
elt_000_06534	CdPbTb ₂ Zn ₂	6	-2.681	-2.853	0.000e+00	0.00438	0.865	1.081
elt_000_06557	Dy ₃ Ga ₃	6	-3.905	-4.227	0.000e+00	0.00484	0.831	0.939
elt_000_06563	Al ₃ Nd ₃	6	-4.151	-4.544	-2.000e-06	0.00364	1.277	1.396
elt_000_06569	Co ₃ GeNiTi	6	-6.432	-6.584	-2.000e-06	0.00592	0.351	0.424
elt_000_06575	AlBaGd ₃ Ge	6	-4.076	-4.222	-1.500e-05	0.00362	0.927	2.81
elt_000_06585	Co ₂ NaPd ₂ SbYb	7	-4.075	-4.619	-3.000e-06	0.00638	1.889	2.483
elt_000_06587	MgNd ₂ Zn ₃	6	-2.378	-2.676	-2.000e-06	0.00705	1.631	2.445
elt_000_06593	CuDy ₂ I ₃ Te	7	-3.552	-3.865	-2.000e-06	0.00966	0.627	0.736
elt_000_06612	AsNaRu ₂	4	-5.12	-5.806	0.000e+00	0.0093	0.742	2.117
elt_000_06655	LiSbSiTb ₃	6	-4.405	-4.759	-7.000e-06	0.00427	0.991	1.174
elt_000_06670	Br ₃ Dy ₂ FeSn	7	-4.168	-4.294	-2.000e-06	0.00625	0.638	0.773
elt_000_06689	Nd ₂ Sn ₂	4	-4.411	-5.03	-1.000e-06	0.00518	1.357	1.892
elt_000_06696	AuGaGeNd ₃ Sr	7	-4.177	-4.298	-9.000e-06	0.00719	0.376	0.38
elt_000_06700	Dy ₂ Sb ₃ Sm	6	-4.576	-5.28	-1.000e-06	0.0035	0.918	1.206
elt_000_06724	Ga ₂ Tb ₄	6	-4.078	-4.375	1.000e-06	0.0064	0.952	0.863
elt_000_06768	CePtRu ₂	4	-7.452	-7.825	-3.000e-06	0.00789	0.795	0.58
elt_000_06812	Dy ₂ GePt ₃	6	-5.839	-6.244	0.000e+00	0.00569	1.116	1.049
elt_000_06831	Nd ₂ Pt ₂ Te ₂	6	-5.065	-5.647	-1.000e-06	0.00698	1.419	2.834
elt_000_06847	DyNiTb ₂ Zn	5	-4.073	-4.194	-4.000e-06	0.00342	0.358	0.461
elt_000_06861	As ₂ OsPRu ₂ Sc	7	-6.823	-7.467	0.000e+00	0.00923	0.584	0.865
elt_000_06864	GeMn ₂ OsSi ₂	6	-7.101	-7.485	0.000e+00	0.00723	0.785	0.634
elt_000_06877	CdCo ₂ Nd ₃ Sn ₂	8	-4.582	-4.826	-1.000e-06	0.00637	0.53	0.731
elt_000_06922	Gd ₂ SbSe ₄ W	8	-5.269	-5.739	-2.000e-06	0.00472	0.517	0.668
elt_000_06923	BiGd ₃ GePt	6	-5.095	-5.523	0.000e+00	0.0029	0.997	1.299
elt_000_06936	AsGd ₂ KP ₃	7	-4.493	-5.313	-2.000e-06	0.00575	0.891	2.176
elt_000_06947	AgCaGaYb ₂ Zn	6	-2.018	-2.237	1.000e-06	0.00796	1.585	2.938
elt_000_06949	BaGd ₃ PdSn ₂	7	-4.528	-4.656	-1.000e-06	0.00423	0.3	0.497
elt_000_06965	Dy ₂ IrPbSb	5	-4.897	-5.662	0.000e+00	0.00568	1.258	0.92
elt_000_06980	As ₃ ReRu ₂	6	-6.947	-7.333	-1.000e-06	0.0061	0.576	0.629
elt_000_07000	Ge ₄ Ru ₂ Y	7	-5.289	-6.34	-2.000e-06	0.00895	0.85	0.948
elt_000_07003	AsDy ₂ GeTe	5	-4.577	-5.138	-2.000e-06	0.00649	1.283	1.252
elt_000_07006	Ru ₂ Sn ₂ Y ₂	6	-5.962	-6.811	-2.000e-06	0.00311	0.657	0.782
elt_000_07020	BaGa ₃ Gd ₂	6	-3.463	-3.658	0.000e+00	0.00561	0.812	0.92
elt_000_07053	CRu ₂ Y	4	-7.683	-8.582	0.000e+00	0.00332	1.012	1.268
elt_000_07102	Fe ₂ Gd ₂ I ₂	6	-4.359	-4.706	0.000e+00	0.00643	1.002	1.328
elt_000_07107	Nd ₂ Sb ₂ SrZn	6	-3.713	-4.043	-6.000e-06	0.00485	1.118	1.723
elt_000_07111	Dy ₃ Ga ₃	6	-3.889	-4.229	-1.000e-06	0.00802	0.915	1.156
elt_000_07134	CrGd ₂ Sn ₂ TeW ₂	8	-6.2	-6.816	0.000e+00	0.00562	0.742	0.873
elt_000_07137	As ₃ CrMn ₂	6	-6.533	-6.822	-8.000e-06	0.00464	0.399	0.58
elt_000_07156	BaCINSiTb ₂	6	-4.666	-5.272	-2.000e-05	0.00458	0.892	0.826
elt_000_07165	AuCsHgYb ₂	5	-1.566	-1.843	-2.450e-05	0.00328	1.145	1.786
elt_000_07202	Dy ₃ Sn ₃	6	-4.253	-4.762	-3.000e-06	0.00665	0.99	1.202
elt_000_07206	Cd ₂ NiTb ₃	6	-3.517	-3.617	-1.000e-06	0.00719	0.365	0.422
elt_000_07235	AsGeNiPRu ₂ Tb	7	-6.229	-6.718	-9.000e-06	0.00688	0.706	0.662
elt_000_07239	ErMoNdSbTb ₂	6	-5.332	-5.746	-1.000e-06	0.00451	1.068	1.689
elt_000_07241	Fe ₂ MnP ₃	6	-6.827	-7.123	-3.200e-05	0.0061	0.529	0.614

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_07296	Co ₂ Ge ₂ Sn ₂	6	-4.739	-5.104	-7.000e-06	0.00874	0.978	1.328
elt_000_07300	Fe ₃ HfTcV	6	-8.463	-8.854	-4.800e-05	0.00686	0.55	0.731
elt_000_07320	Gd ₂ LaNiSb ₂ Si	7	-5.177	-5.65	8.000e-06	0.00992	0.931	1.253
elt_000_07324	Pt ₃ Ru ₂ Zn	6	-5.558	-6.296	1.000e-06	0.00666	0.561	0.609
elt_000_07327	GaNd ₄ NiRu	7	-5.268	-5.431	3.000e-06	0.00965	0.92	1.379
elt_000_07329	BaSb ₃ Tb ₂	6	-4.314	-4.863	-2.000e-06	0.00452	1.141	1.942
elt_000_07334	Al ₂ EuGeTb ₂	6	-3.822	-4.244	-1.000e-06	0.00478	1.681	2.716
elt_000_07346	Co ₂ GaSSnTb ₃	8	-5.11	-5.282	-6.000e-06	0.00644	0.699	1.13
elt_000_07378	GaLaNd ₂ Si ₂	6	-4.826	-5.196	-2.600e-05	0.00719	0.783	1.917
elt_000_07386	Gd ₂ PtRbSn	5	-4.209	-4.354	-2.000e-06	0.00528	0.337	0.416
elt_000_07398	Ni ₃ PTb ₃	7	-5.162	-5.621	-1.500e-05	0.00618	0.983	1.036
elt_000_07403	Ga ₂ Tb ₄	6	-4.07	-4.381	-1.000e-06	0.00746	0.603	0.776
elt_000_07406	PbSeYb ₂	4	-2.561	-3.645	0.000e+00	0.00295	1.978	3.219
elt_000_07433	Gd ₂ Si ₂ Sr	5	-4.216	-4.565	-1.000e-06	0.00487	0.599	0.776
elt_000_07458	CrGd ₂ Si ₅	8	-5.412	-5.967	-2.000e-06	0.0064	0.827	1.418
elt_000_07491	CrCu ₂ Dy ₃ Sb	7	-4.954	-5.038	3.000e-06	0.00444	0.523	0.672
elt_000_07493	Dy ₂ Te ₅ U	8	-5.383	-5.47	-2.930e-04	0.00394	0.728	1.796
elt_000_07498	GaLi ₂ MgNiTb ₂ Ti	8	-3.669	-3.84	-7.000e-06	0.00959	0.828	1.064
elt_000_07501	KNd ₂ Tl	4	-2.827	-3.111	1.000e-06	0.00202	1.496	1.149
elt_000_07506	Dy ₂ GaPtPuRh	6	-6.659	-6.94	2.330e-04	0.00634	0.509	0.726
elt_000_07527	As ₃ PPtRu ₂	7	-5.99	-6.465	-3.000e-06	0.00684	0.791	0.798
elt_000_07534	Dy ₂ FeMgSbTe ₂	7	-4.489	-4.681	-1.000e-06	0.00317	0.464	0.606
elt_000_07536	Sb ₂ SnTb ₂ Te	6	-4.344	-4.788	-1.000e-06	0.00295	1.341	1.582
elt_000_07564	Ge ₂ La ₂ MgTb ₂	7	-4.268	-4.643	-1.000e-06	0.00953	0.781	1.308
elt_000_07578	Fe ₃ GaSiTh	6	-5.764	-6.593	-8.000e-06	0.00466	0.617	1.697
elt_000_07597	Hg ₂ RbSbYb ₂	6	-1.611	-1.844	-7.000e-06	0.00566	1.296	3.976
elt_000_07598	Dy ₂ PbTl	4	-3.622	-4.097	1.000e-06	0.00407	1.048	1.12
elt_000_07602	AlMn ₃ Si ₂	6	-6.664	-7.08	2.000e-06	0.00468	0.809	1.806
elt_000_07610	GeNd ₂ PtSSr	6	-4.873	-5.302	-3.000e-06	0.0033	0.914	2.267
elt_000_07611	AsMn ₂ RhU	5	-7.834	-8.362	-1.000e-06	0.00991	1.295	1.412
elt_000_07630	Dy ₃ PPt ₂	6	-5.863	-6.403	-2.600e-05	0.00619	0.686	0.892
elt_000_07643	GeMn ₂ PtSbSc	6	-6.251	-6.592	-5.000e-06	0.00376	1.207	1.731
elt_000_07651	Fe ₂ Pt ₃ Si	6	-6.472	-6.818	-2.100e-05	0.00797	0.465	0.638
elt_000_07683	AgGd ₂ Ge ₂ Sr	6	-3.836	-4.226	0.000e+00	0.00574	0.652	0.901
elt_000_07684	Ge ₂ Tb ₃ Zn	6	-4.18	-4.504	-2.000e-06	0.00396	0.789	0.769
elt_000_07693	PtSi ₃ Tb ₃ Ti	8	-5.724	-5.988	1.000e-06	0.00697	0.757	1.26
elt_000_07714	Al ₃ MgYb ₃ Zn	8	-2.173	-2.386	-2.200e-05	0.00229	1.032	0.983
elt_000_07717	Yb ₃ Zn ₃	6	-1.344	-1.561	-6.000e-07	0.00315	1.718	3.487
elt_000_07739	AlCeCrDy ₂ Si ₂	7	-5.577	-5.802	0.000e+00	0.00883	0.694	0.858
elt_000_07740	AlGeRhSnYb ₃	7	-3.719	-3.987	0.000e+00	0.00323	1.206	2.75
elt_000_07748	Gd ₄ Ge ₂ Pd ₂	8	-5.222	-5.456	0.000e+00	0.0051	0.717	1.257
elt_000_07757	AuMgSn ₂ Yb ₂	6	-2.845	-3.039	-5.000e-06	0.00499	0.623	0.803
elt_000_07762	GaRbS ₃ Tb ₂	7	-4.215	-4.94	-3.000e-06	0.00429	1.532	1.868
elt_000_07774	CaGe ₂ PdRu ₂	6	-4.957	-5.903	-4.000e-06	0.00739	0.538	0.367
elt_000_07780	Si ₃ Tb ₃	6	-5.103	-5.551	-2.000e-06	0.00375	0.692	1.789
elt_000_07782	As ₂ Co ₂ FeW	6	-6.768	-7.276	-4.200e-05	0.00937	0.443	0.521
elt_000_07783	GeSi ₂ Tb ₃	6	-4.97	-5.524	-2.000e-06	0.00347	0.806	1.284
elt_000_07785	Gd ₃ Si ₃	6	-5.164	-5.57	2.000e-06	0.00332	0.498	0.85
elt_000_07792	Dy ₃ InSi ₂	6	-4.732	-5.076	-1.000e-06	0.00488	0.656	0.904
elt_000_07795	Al ₃ Tb ₃	6	-4.155	-4.496	0.000e+00	0.00298	1.095	1.351
elt_000_07816	CaGaMoPRuTb ₂	7	-5.605	-5.988	1.000e-06	0.0078	1.144	1.24
elt_000_07835	As ₄ Nd ₃	7	-5.026	-5.695	-5.000e-06	0.00543	1.072	1.518

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_07840	I ₄ Nd ₂	6	-3.743	-3.869	-3.000e-06	0.00573	0.498	0.495
elt_000_07852	Dy ₃ Ga ₂ NiSb	7	-4.389	-4.653	0.000e+00	0.00554	0.675	0.698
elt_000_07858	AlCo ₂ Gd ₃ P	7	-5.339	-5.808	-6.000e-06	0.00706	1.137	2.309
elt_000_07867	CuGaTb ₃	5	-4.071	-4.226	-4.000e-06	0.00362	0.359	1.675
elt_000_07877	Ru ₂ Th	3	-7.794	-8.53	-1.000e-06	0.00408	1.026	0.638
elt_000_07878	Dy ₂ RbZn ₃	6	-1.975	-2.167	-2.000e-06	0.00469	1.294	1.93
elt_000_07891	As ₂ CeRu ₃ Si	7	-6.723	-7.364	5.000e-06	0.00844	0.686	1.653
elt_000_07951	CdKNd ₂ Pd	5	-3.238	-3.403	-3.000e-06	0.00655	0.755	2.306
elt_000_08042	Au ₄ Tb ₂	6	-3.964	-4.435	0.000e+00	0.00256	1.466	1.283
elt_000_08062	Au ₄ Ru ₂	6	-4.666	-4.966	1.000e-06	0.0048	0.508	1.752
elt_000_08079	BMoRu ₂ SiYbZr	7	-7.253	-7.498	0.000e+00	0.00624	0.52	0.378
elt_000_08084	Ge ₂ PdPt ₂ Tb ₂	7	-5.541	-5.932	-2.300e-05	0.00888	0.966	2.491
elt_000_08091	RuSn ₃ Tb ₂ Zn	7	-4.288	-4.863	-1.000e-06	0.00625	0.906	1.165
elt_000_08094	Co ₄ NiV	6	-6.91	-7.007	-6.000e-06	0.00884	0.071	0.183
elt_000_08098	Dy ₂ GdMnSi ₃	7	-5.5	-5.938	-2.100e-05	0.00986	0.68	0.71
elt_000_08100	GaNd ₄ Pt ₂	7	-5.269	-5.605	-1.000e-06	0.00775	0.267	0.668
elt_000_08102	Ga ₃ Nd ₃	6	-4.002	-4.292	-4.900e-05	0.00636	0.88	2.107
elt_000_08115	Nd ₂ Sb ₃ Sr	6	-4.11	-4.953	-1.000e-06	0.00483	1.074	1.624
elt_000_08122	P ₂ Ru ₂ Zn ₂	6	-5.01	-5.599	-2.000e-06	0.00392	0.889	1.163
elt_000_08189	As ₃ FeI ₂ Yb ₂	8	-3.353	-4.128	0.000e+00	0.00412	0.783	1.452
elt_000_08215	AuMn ₂ Sb	4	-5.1	-5.884	-3.000e-06	0.00694	0.891	1.085
elt_000_08218	AsCuDy ₂ ITe	6	-3.949	-4.458	-5.000e-06	0.00663	0.861	2.262
elt_000_08236	As ₂ GeNd ₂ Ni ₂ Sn	8	-4.99	-5.447	-2.000e-06	0.00472	1.326	2.253
elt_000_08246	CuGaGd ₂ O ₈ Tl	6	-4.519	-5.042	-1.600e-05	0.00716	1.03	1.787
elt_000_08249	Fe ₂ Ni ₃ Si	6	-6.328	-6.443	-2.000e-05	0.00714	0.177	0.214
elt_000_08256	Ba ₂ CdIrSbSnYb ₂	8	-3.276	-3.606	-3.000e-06	0.00536	1.73	2.536
elt_000_08258	Fe ₂ Mn ₂ NdSi	6	-6.642	-7.185	-4.000e-06	0.00616	0.729	0.619
elt_000_08274	Ga ₂ Gd ₃ Ni ₂	7	-4.58	-4.646	1.000e-06	0.00694	0.223	0.352
elt_000_08275	Ga ₂ Nd ₂ Sm	5	-4.118	-4.303	-4.000e-06	0.00644	0.709	2.313
elt_000_08282	Dy ₃ Si ₃	6	-5.136	-5.535	-1.000e-06	0.00476	0.545	0.865
elt_000_08299	As ₄ Gd ₂ W	7	-6.028	-6.395	-5.000e-06	0.00574	1.019	3.018
elt_000_08306	Dy ₂ PbSbScSrTe	7	-4.333	-4.597	0.000e+00	0.00524	0.98	2.389
elt_000_08312	Co ₃ Sn ₂ Yb ₃	8	-4.064	-4.325	1.000e-06	0.00479	0.625	0.597
elt_000_08334	AlGaSnTb ₂	5	-3.931	-4.488	-1.000e-06	0.00781	1.337	1.691
elt_000_08342	GaLiMn ₂	4	-5.27	-5.499	-1.000e-06	0.00537	0.458	1.471
elt_000_08351	Ce ₂ Ru ₂ SbSn	6	-6.115	-6.812	2.000e-06	0.00772	1.183	0.858
elt_000_08373	As ₂ Ru ₂ Sb ₂	6	-5.846	-6.059	0.000e+00	0.00537	0.711	0.827
elt_000_08383	Dy ₂ Ga ₂ GeYb	6	-3.599	-3.958	-1.300e-05	0.00723	0.761	0.858
elt_000_08396	AuRu ₂ SiSnTi ₂	7	-6.472	-6.904	1.000e-06	0.00464	0.899	1.229
elt_000_08397	As ₂ DyGd ₂ Ni ₂	7	-5.292	-5.449	9.000e-06	0.00671	0.643	0.865
elt_000_08410	Ag ₂ BiTb ₂ Tl	6	-3.352	-3.764	-2.000e-06	0.00444	1.459	1.36
elt_000_08415	AlDyGa ₂ Gd ₂	6	-4.053	-4.362	-1.000e-05	0.00506	0.86	0.93
elt_000_08431	Ga ₂ NiTb ₄	7	-4.474	-4.6	-3.000e-06	0.00419	0.508	0.689
elt_000_08437	Cl ₄ Ru ₂	6	-3.705	-4.389	-1.000e-06	0.00874	0.627	0.993
elt_000_08442	Dy ₃ Si ₄	7	-5.093	-5.762	-1.000e-06	0.00438	0.963	3.608
elt_000_08444	Dy ₃ Ga ₂ Hg	6	-3.417	-3.715	0.000e+00	0.00516	1.033	1.52
elt_000_08482	Ga ₂ Gd ₂ Si ₂	6	-4.482	-4.83	-1.000e-06	0.00482	1.247	1.897
elt_000_08492	Ga ₂ PdYb ₃	6	-2.801	-3.158	-3.000e-06	0.00336	1.488	2.61
elt_000_08515	AuGa ₂ Gd ₂ Sr	6	-3.513	-3.759	-6.000e-06	0.00628	0.679	0.738
elt_000_08518	Dy ₂ GeLaSn ₂ Te	7	-4.307	-4.78	2.000e-06	0.00606	0.816	0.921
elt_000_08557	GaGd ₃ Te ₂	6	-4.277	-4.713	2.000e-06	0.0041	1.114	1.716
elt_000_08590	AuSbYb ₄	6	-2.678	-2.821	-2.000e-06	0.00746	0.59	0.722

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_08595	BaBiSbSnYb ₂	6	-3.135	-3.528	0.000e+00	0.00404	1.082	1.793
elt_000_08597	Ga ₃ Gd ₃ Ni ₂	8	-4.563	-4.625	1.000e-06	0.00983	0.699	0.988
elt_000_08601	Dy ₂ IMgSb ₂	6	-3.461	-4.11	0.000e+00	0.00386	1.007	1.46
elt_000_08606	AuGd ₂ PrSi ₂	6	-4.901	-5.307	0.000e+00	0.00349	1.09	1.231
elt_000_08624	CrGeRu ₂ ScTi	6	-7.469	-7.902	-1.000e-05	0.00856	0.322	0.347
elt_000_08629	Gd ₃ Sn ₃	6	-4.46	-4.819	3.000e-06	0.00834	0.799	1.131
elt_000_08631	AgS ₂ SnYb ₃	7	-3.424	-4.016	0.000e+00	0.00435	1.596	3.148
elt_000_08661	Au ₃ LaTb ₂	6	-4.352	-4.779	1.000e-06	0.00963	1.42	2.411
elt_000_08673	AlDy ₃ Ga ₂	6	-3.89	-4.305	-1.000e-06	0.00907	0.825	0.951
elt_000_08683	BaGe ₂ Nd ₃ Os	7	-5.403	-5.625	-1.900e-05	0.00871	0.657	0.686
elt_000_08691	CrGa ₃ Gd ₂ Pr	7	-4.475	-4.794	-1.000e-06	0.0071	1.285	2.59
elt_000_08696	FeGa ₃ Gd ₂ SnTm	8	-4.525	-4.582	0.000e+00	0.00953	0.279	0.291
elt_000_08715	Cu ₂ Nd ₃ Zn	6	-3.623	-3.9	-8.800e-05	0.00631	0.587	0.713
elt_000_08744	CdPdSb ₂ Tb ₂ Zn	7	-3.814	-4.025	0.000e+00	0.00518	0.801	1.405
elt_000_08752	ErNi ₂ Sn ₂ Tb ₂	7	-4.862	-5.02	-1.000e-06	0.00716	0.376	0.306
elt_000_08776	NbTe ₄ Yb ₂	7	-4.029	-4.37	0.000e+00	0.00834	1.546	3.678
elt_000_08792	Mn ₂ PPtSbSc	6	-6.459	-6.916	-1.500e-05	0.00648	0.661	0.873
elt_000_08822	CoGa ₂ Nd ₃	6	-4.453	-4.865	-7.000e-06	0.0043	1.205	2.388
elt_000_08835	Dy ₂ PdRbSb	5	-3.962	-4.163	-3.000e-06	0.00338	0.289	0.463
elt_000_08845	Au ₂ Nd ₃ Sn	6	-4.509	-4.757	-1.000e-06	0.00431	0.907	1.236
elt_000_08847	CeDy ₂ Si ₃	6	-5.321	-5.73	-2.000e-06	0.00645	0.981	1.144
elt_000_08857	AsCrFe ₂ GePt	6	-6.405	-6.859	-1.100e-05	0.00687	0.375	0.616
elt_000_08859	AlGeRu ₂ Sn ₂	6	-5.226	-5.806	-3.000e-06	0.00645	0.665	0.532
elt_000_08868	AgCaNd ₂	4	-3.251	-3.602	3.000e-06	0.00275	1.268	1.137
elt_000_08871	Sb ₃ Tb ₃	6	-4.506	-5.504	0.000e+00	0.00439	1.15	2.027
elt_000_08878	Gd ₃ Ge ₃ Ni ₂	8	-5.019	-5.493	-3.000e-06	0.00688	1.249	2.496
elt_000_08883	Dy ₂ Ga ₂ Sr	5	-3.331	-3.537	-1.000e-05	0.00705	0.796	2.131
elt_000_08908	BrCdGd ₂ S ₂	6	-4.43	-4.637	-1.000e-06	0.00427	0.435	1.424
elt_000_08918	Si ₃ Tb ₃	6	-5.101	-5.551	-6.000e-06	0.00553	0.72	1.844
elt_000_08946	CoGa ₂ Gd ₃	6	-4.476	-4.844	-1.000e-06	0.00762	1.068	1.399
elt_000_08968	Ga ₂ Gd ₃ Ge	6	-4.231	-4.556	1.000e-06	0.00657	0.721	0.874
elt_000_08978	AlGd ₃ PbSmZn ₂	8	-3.449	-3.809	-4.000e-06	0.00707	0.955	1.416
elt_000_09004	CaGeP ₄ Tb ₂	8	-4.854	-5.413	0.000e+00	0.00511	1.118	1.748
elt_000_09007	Ga ₂ Nd ₃ Sn	6	-4.096	-4.516	0.000e+00	0.00472	0.735	1.068
elt_000_09044	FeLaRu ₂ Si ₂	6	-6.898	-7.213	-1.000e-06	0.0045	0.24	0.304
elt_000_09069	Ge ₃ Tb ₃	6	-4.758	-5.172	-4.000e-06	0.00864	0.637	0.877
elt_000_09098	ClGd ₂ PtRb	5	-3.698	-4.553	0.000e+00	0.0045	2.246	3.303
elt_000_09129	Gd ₃ Pt ₃ SnTe	8	-5.235	-5.734	0.000e+00	0.00321	0.832	1.186
elt_000_09130	Dy ₃ Ga ₂ Ni	6	-4.364	-4.646	0.000e+00	0.00396	0.997	1.029
elt_000_09132	As ₂ GeNd ₃	6	-5.121	-5.686	-1.000e-06	0.00744	0.821	1.005
elt_000_09137	Si ₃ Tb ₃	6	-4.961	-5.551	0.000e+00	0.0072	0.65	1.866
elt_000_09147	Co ₃ GaTi ₂	6	-6.448	-6.863	-6.000e-06	0.00702	1.182	1.978
elt_000_09152	AuBaDy ₂ Ga ₃	7	-3.501	-3.742	0.000e+00	0.00403	0.786	0.905
elt_000_09154	AgAlCuTb ₃	6	-3.876	-4.229	-3.000e-06	0.00588	1.613	2.717
elt_000_09158	Rh ₂ Tb ₅	7	-5.473	-5.751	-3.000e-06	0.00292	1.118	1.512
elt_000_09177	AsBiDy ₂ Te ₄	8	-4.196	-4.535	-2.000e-06	0.0062	1.02	2.452
elt_000_09200	CdGaGd ₃ PtSi	7	-4.441	-4.777	0.000e+00	0.00426	0.808	0.975
elt_000_09205	NdRu ₂ Sn ₂ Tb	6	-3.636	-6.009	0.000e+00	0.00468	0.68	0.545
elt_000_09212	Gd ₂ PtRbTe	5	-3.896	-4.555	-1.400e-05	0.00637	1.289	1.521
elt_000_09214	CaGe ₃ Tb ₂	6	-4.293	-4.678	-3.000e-05	0.00771	0.682	0.846
elt_000_09217	As ₃ Dy ₂ Pr	6	-5.111	-5.835	1.000e-06	0.00298	0.805	1.129
elt_000_09248	Co ₃ Ge ₃	6	-5.294	-5.814	-1.300e-05	0.00554	0.855	1.3

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_09250	Dy ₂ I ₃ Rh	6	-3.85	-4.439	-4.000e-06	0.00587	0.254	2.712
elt_000_09256	As ₂ Fe ₂ Ge ₂	6	-5.368	-5.728	-6.000e-06	0.00947	0.667	0.939
elt_000_09264	Gd ₃ Ni ₂ Sb ₂	7	-4.986	-5.261	0.000e+00	0.00552	0.857	0.75
elt_000_09270	AsCl ₃ Mn ₂	6	-3.932	-4.829	-4.000e-06	0.00474	0.62	0.803
elt_000_09275	GePt ₂ SiTb ₂ Y	7	-5.978	-6.346	0.000e+00	0.00388	1.174	1.51
elt_000_09276	Al ₆ Nd ₂	8	-3.711	-4.342	0.000e+00	0.00484	0.969	2.023
elt_000_09283	OsSbSn ₂ Tb ₃	7	-5.427	-5.618	-2.000e-06	0.00716	0.567	0.811
elt_000_09295	CCoGeRu ₂ Th	6	-7.184	-7.776	-1.300e-05	0.00719	1.044	2.138
elt_000_09296	CoDy ₃ Ga ₂	6	-4.36	-4.715	0.000e+00	0.0044	0.483	0.901
elt_000_09307	As ₄ Dy ₂ FeI	8	-4.621	-5.104	-1.200e-05	0.00741	0.722	1.976
elt_000_09309	Ga ₂ GeNd ₃	6	-4.238	-4.569	-1.000e-05	0.00651	0.675	0.849
elt_000_09314	NbRu ₂ Tb ₂ Te ₃	8	-6.17	-6.401	-2.000e-06	0.0077	0.637	0.939
elt_000_09326	AgAlCuNd ₃	6	-3.923	-4.264	-3.000e-06	0.00448	1.651	2.207
elt_000_09331	Nd ₄ Rh ₂	6	-5.713	-5.925	0.000e+00	0.00399	0.622	0.716
elt_000_09338	As ₂ P ₂ Ru ₂	6	-6.007	-6.537	1.000e-06	0.00409	0.585	1.932
elt_000_09349	Ga ₃ Tb ₃	6	-3.839	-4.241	-2.000e-06	0.00317	0.792	0.948
elt_000_09354	As ₂ Dy ₂ Fe ₃ I	8	-5.591	-5.985	0.000e+00	0.00592	1.109	2.739
elt_000_09359	Dy ₂ Hg ₄ Sb	7	-2.111	-2.37	-3.000e-06	0.00386	1.27	2.435
elt_000_09378	Yb ₃ Zn ₄	7	-1.335	-1.427	-5.400e-06	0.00366	1.149	2.217
elt_000_09379	AgGeMgNd ₂ Pd	6	-4.079	-4.263	0.000e+00	0.00541	0.314	0.552
elt_000_09380	CuGd ₂ Se ₃	6	-4.641	-5.239	-3.000e-06	0.00675	1.058	1.711
elt_000_09406	As ₂ BaCdGd ₂ Ni ₂	8	-4.389	-4.621	-2.000e-06	0.00703	1.05	3.547
elt_000_09411	Dy ₂ MgPt ₃ Te	7	-5.023	-5.288	-1.200e-05	0.00433	0.376	0.808
elt_000_09416	Hg ₂ PbYb ₃	6	-1.735	-2.026	-1.000e-06	0.00344	1.187	2.143
elt_000_09429	Ba ₂ Mn ₂ P ₃	7	-5.298	-6.172	-2.000e-06	0.00756	0.706	1.251
elt_000_09433	AlCaGePt ₂ Tb ₂	7	-4.974	-5.331	0.000e+00	0.00306	1.439	1.595
elt_000_09504	AlFe ₃ Hf ₂	6	-7.706	-8.09	6.000e-06	0.00579	0.468	2.593
elt_000_09506	AsPtSb ₂ SnTb ₂	7	-4.83	-5.224	0.000e+00	0.00412	1.765	2.369
elt_000_09518	Ru ₃ Y	4	-7.901	-8.354	0.000e+00	0.0078	0.655	0.938
elt_000_09522	Ni ₂ P ₂ W ₂	6	-7.629	-8.169	-1.000e-06	0.00505	0.502	0.947
elt_000_09532	Dy ₂ GeLuSbTeZn	7	-4.076	-4.558	0.000e+00	0.0072	1.516	2.645
elt_000_09564	AlGa ₂ Tb ₃	6	-3.97	-4.306	0.000e+00	0.0047	0.911	0.982
elt_000_09624	Cd ₃ Gd ₂ Sr	6	-2.066	-2.375	0.000e+00	0.00338	0.639	2.568
elt_000_09635	Gd ₃ MnTe ₃	7	-5.032	-5.404	-4.000e-06	0.00941	1.073	3.194
elt_000_09657	Se ₄ Yb ₄	8	-4.036	-4.503	-4.000e-06	0.00469	1.039	2.137
elt_000_09659	Br ₂ Dy ₂ Ru ₂	6	-4.803	-5.822	-3.000e-06	0.00683	1.573	2.013
elt_000_09660	Gd ₂ Rb ₂ Te ₂	6	-3.388	-3.568	-4.000e-06	0.00266	0.762	0.793
elt_000_09670	Ge ₂ Ru ₂ Tb ₂ Te	7	-5.628	-6.21	-8.000e-06	0.0081	1.034	0.822
elt_000_09675	Ga ₃ Tb ₃	6	-3.947	-4.242	-5.000e-06	0.00842	0.832	0.832
elt_000_09687	AlNd ₂ RhSb ₂	6	-5.047	-5.514	0.000e+00	0.00689	1.237	2.968
elt_000_09707	Ga ₃ Nd ₃	6	-3.978	-4.292	-2.000e-06	0.00277	0.929	1.964
elt_000_09710	AlDy ₃ Ge ₂	6	-4.859	-4.991	-2.000e-06	0.00864	0.812	0.899
elt_000_09713	Ga ₃ Nd ₃	6	-4.031	-4.291	-2.000e-06	0.00354	0.854	1.003
elt_000_09717	AsCuGd ₃ MnMo	7	-5.724	-6.174	1.000e-06	0.00562	0.604	1.239
elt_000_09724	Ga ₃ Nd ₃	6	-3.956	-4.289	-3.000e-06	0.0076	0.814	0.749
elt_000_09751	RuTe ₂ Yb ₂	5	-3.623	-4.529	8.000e-06	0.00641	1.842	2.238
elt_000_09761	Dy ₂ Se ₄ Te	7	-4.714	-4.936	0.000e+00	0.00506	0.537	2.686
elt_000_09765	AlGd ₃ Si ₂	6	-4.867	-5.29	-1.000e-06	0.00282	0.867	1.083
elt_000_09784	Ga ₂ Yb ₃ Zn	6	-2.004	-2.24	1.000e-06	0.0075	1.181	1.332
elt_000_09799	AlAsCo ₃ W	6	-6.797	-7.04	-1.000e-06	0.00601	0.496	0.552
elt_000_09811	InNaSb ₂ Yb ₂	6	-2.909	-3.088	-3.000e-06	0.00469	0.88	1.071
elt_000_09866	As ₃ Dy ₂ Te	6	-4.588	-5.235	-1.000e-06	0.00284	1.653	2.259

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_09909	FeHfTe ₃ Yb ₂	7	-4.906	-5.154	-4.000e-06	0.00533	1.035	1.358
elt_000_09932	CsGd ₂ GeSe ₃	7	-3.977	-4.788	0.000e+00	0.00301	1.02	1.746
elt_000_09947	AgNd ₂ Se ₄	7	-4.607	-4.921	3.000e-06	0.00474	0.832	0.77
elt_000_09952	CaGd ₂ Ge ₂ Sb	6	-4.282	-4.769	-4.000e-06	0.00649	0.527	0.881
elt_000_09976	Nd ₂ Sn ₃ Yb	6	-3.908	-4.379	-1.000e-06	0.00685	1.626	2.981
elt_000_09986	AgGaGeRu ₂	5	-5.362	-5.64	0.000e+00	0.00758	0.443	0.593
elt_000_09995	GeInRu ₂ TeTm	6	-5.494	-5.686	1.000e-06	0.0082	0.352	0.596
elt_000_10001	I ₂ MoOsTb ₂	6	-5.115	-5.942	0.000e+00	0.00592	1.525	2.533
elt_000_10035	CdLaNd ₂	4	-3.587	-3.899	9.000e-06	0.00851	1.141	0.793
elt_000_10055	Sb ₂ SrTb ₂	5	-3.907	-4.56	-6.000e-06	0.00629	1.063	1.491
elt_000_10075	Ga ₃ SrYb ₂	6	-2.369	-2.594	-3.000e-06	0.00796	0.99	1.768
elt_000_10113	Al ₃ Nd ₂ Sb	6	-4.227	-4.579	-2.000e-06	0.00265	0.856	0.947
elt_000_10115	CeGe ₃ Ru ₂	6	-6.27	-6.601	1.000e-06	0.00879	0.754	0.965
elt_000_10120	CoGd ₂ Ge ₅	8	-4.918	-5.332	-1.000e-06	0.00624	0.806	1.187
elt_000_10124	Ag ₂ CaSbTb ₂	6	-3.539	-3.861	-2.000e-06	0.00287	0.993	1.1
elt_000_10125	Fe ₂ Nd ₅	7	-5.49	-5.623	-1.100e-05	0.00814	0.255	0.467
elt_000_10136	Si ₂ Tb ₄ Zn	7	-4.383	-4.646	-2.000e-06	0.00281	0.445	0.914
elt_000_10145	AsAuMgNi ₃	6	-3.919	-4.468	-1.100e-05	0.00642	0.777	0.938
elt_000_10148	FePtRu ₂ ScSi	6	-7.562	-7.702	1.400e-05	0.00672	0.179	0.229
elt_000_10154	Ga ₂ GeNd ₃	6	-4.307	-4.57	7.000e-06	0.00669	0.707	0.778
elt_000_10159	CdNi ₂ Sb ₂ Zr	6	-4.598	-4.996	0.000e+00	0.00891	0.959	1.122
elt_000_10182	As ₄ Cr ₂ Dy ₂	8	-5.781	-6.38	-2.300e-05	0.0052	1.474	3.375
elt_000_10197	CoFe ₂ Ga ₃	6	-5.118	-5.281	-1.800e-05	0.00833	0.101	0.243
elt_000_10224	AsCoCrHf ₂ Ru ₂	7	-8.229	-8.688	1.000e-06	0.00508	1.116	2.013
elt_000_10225	Ga ₃ Gd ₃	6	-3.934	-4.254	0.000e+00	0.00622	1.087	1.286
elt_000_10230	Al ₃ Ru ₂ Ti	6	-6.504	-6.616	3.000e-06	0.0088	0.09	0.24
elt_000_10244	Dy ₂ Fe ₂ SeTe ₃	8	-5.012	-5.264	-6.000e-06	0.00533	1.016	2.25
elt_000_10246	Ni ₃ SbSi ₂ ZnZr	8	-5.159	-5.477	1.000e-06	0.00831	0.724	0.965
elt_000_10266	Co ₂ GeTb ₃	6	-5.243	-5.723	2.000e-06	0.00488	1.175	0.906
elt_000_10268	Gd ₂ OsPrSe	5	-5.645	-6.308	0.000e+00	0.00493	1.912	1.931
elt_000_10270	AsCo ₃ ReSn	6	-6.407	-6.775	2.000e-06	0.00701	0.436	0.522
elt_000_10294	AlDy ₃ GaPt	6	-4.469	-5.009	1.000e-06	0.00534	1.392	1.421
elt_000_10304	Al ₂ CoDy ₃	6	-4.667	-4.878	-4.000e-06	0.0065	0.479	1.576
elt_000_10320	Ni ₃ Zr ₃	6	-6.604	-7.253	-2.000e-06	0.00646	1.162	1.038
elt_000_10330	MgSn ₂ Yb ₃	6	-2.439	-2.686	0.000e+00	0.00459	1.284	2.352
elt_000_10338	CuGaNd ₃	5	-4.2	-4.301	1.000e-06	0.00507	0.356	1.781
elt_000_10339	As ₄ Ru ₂	6	-6.081	-6.262	-3.000e-06	0.0061	0.633	1.195
elt_000_10340	AuNi ₂ SnTi ₂	6	-5.394	-5.813	-1.100e-05	0.00638	1.07	2.07
elt_000_10345	Mn ₂ Sb ₄	6	-5.11	-5.528	-4.000e-06	0.00884	0.751	0.918
elt_000_10354	Ge ₅ Nd ₂	7	-4.732	-5.032	4.000e-06	0.00807	0.943	1.099
elt_000_10367	AsMn ₂ Pt	4	-6.61	-7.142	-1.000e-06	0.00314	1.13	2.249
elt_000_10373	CdPdRbTb ₂	5	-3.159	-3.284	-1.000e-06	0.00552	0.589	0.664
elt_000_10384	AgKNd ₂ Sn ₂	6	-3.387	-3.777	0.000e+00	0.00319	1.453	2.008
elt_000_10402	ClGeNd ₂ Te ₃	7	-3.958	-4.641	0.000e+00	0.00581	2.144	3.391
elt_000_10404	AuGe ₂ Mn ₂ Pt	6	-5.647	-5.992	-4.000e-06	0.00489	0.394	2.81
elt_000_10423	CaDy ₂ NiPd	5	-4.325	-4.68	-1.160e-04	0.00654	0.561	0.882
elt_000_10444	As ₃ RhSrTb ₂	7	-4.942	-5.624	0.000e+00	0.00887	0.899	1.599
elt_000_10469	Gd ₃ Ge ₃	6	-4.812	-5.192	0.000e+00	0.00586	0.519	0.666
elt_000_10497	Dy ₃ GaSn ₂	6	-3.889	-4.504	-4.000e-06	0.00503	0.606	0.775
elt_000_10525	GaGd ₂ LaSnTe	6	-4.293	-4.573	-1.000e-06	0.00775	0.763	1.01
elt_000_10537	Ga ₃ Gd ₂ Sr	6	-3.358	-3.66	0.000e+00	0.00692	0.792	1.818
elt_000_10548	Dy ₂ Te ₂ V ₂	6	-5.486	-5.822	2.000e-06	0.00978	0.558	0.543

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_10552	AlCuDy ₂ Nd	5	-4.216	-4.361	1.000e-06	0.00612	0.508	1.66
elt_000_10557	AsCdNd ₃ SbTe	7	-4.354	-4.742	1.000e-06	0.00707	0.917	0.994
elt_000_10575	Ru ₂ Sb ₂ Ti ₂	6	-6.928	-7.32	2.000e-06	0.00409	1.273	2.419
elt_000_10589	Al ₂ Fe ₃ Mo	6	-6.942	-7.153	0.000e+00	0.00687	0.385	0.628
elt_000_10595	Dy ₃ Pd ₃	6	-5.266	-5.702	-3.400e-05	0.00809	0.71	1.891
elt_000_10598	LiNd ₂ NiRuSbTe ₂	8	-4.629	-5.186	0.000e+00	0.00465	1.075	0.908
elt_000_10609	AlGd ₂ LaNi ₃	7	-5.064	-5.266	-5.000e-06	0.0097	0.949	1.118
elt_000_10657	Au ₃ BaYb ₂	6	-2.815	-3.259	0.000e+00	0.00345	1.727	1.938
elt_000_10660	Au ₃ Yb ₃	6	-2.886	-3.259	0.000e+00	0.00357	0.657	0.944
elt_000_10688	AuSb ₂ Tb ₃	6	-4.655	-5.069	0.000e+00	0.00391	0.848	1.62
elt_000_10726	Ga ₃ Tb ₃	6	-3.909	-4.241	-1.000e-06	0.0066	0.873	0.838
elt_000_10733	Au ₃ Gd ₃ Ge ₂	8	-4.573	-4.687	-3.000e-06	0.005	0.391	0.58
elt_000_10742	Al ₃ Nd ₃ NiSm	8	-4.324	-4.771	1.000e-06	0.00706	0.57	0.509
elt_000_10747	Tb ₃ TlZn ₂	6	-3.063	-3.234	-3.200e-05	0.00644	0.969	1.145
elt_000_10748	Co ₂ Dy ₂ FePr	6	-5.572	-5.973	-1.000e-06	0.00973	1.436	2.852
elt_000_10764	AuDy ₃ SnZn	6	-4.012	-4.197	0.000e+00	0.0052	0.896	1.11
elt_000_10765	Gd ₂ PtSbSi ₃ V	8	-5.73	-6.026	-5.000e-06	0.00775	0.651	1.001
elt_000_10774	Ga ₂ ScSnTb ₂	6	-4.336	-4.593	1.000e-06	0.00858	0.668	0.659
elt_000_10813	Gd ₄ GeScSi	7	-5.122	-5.282	1.000e-06	0.00329	0.306	1.446
elt_000_10828	AsGaGe ₂ Nd ₂ Ni	7	-4.763	-5.112	2.000e-06	0.00458	1.178	2.028
elt_000_10853	CrFeNd ₂ Si ₄	8	-5.406	-6.485	-1.000e-05	0.00821	0.675	1.004
elt_000_10856	MgNd ₂ PbSiSr	6	-3.595	-3.918	0.000e+00	0.00717	1.268	1.652
elt_000_10864	Ga ₃ RbTb ₂	6	-3.028	-3.294	-6.000e-06	0.00604	0.726	1.072
elt_000_10877	SnTb ₃ Zn ₃	7	-3.149	-3.273	-1.000e-06	0.00621	0.467	0.489
elt_000_10884	Au ₂ SnYb ₃	6	-3.034	-3.327	-4.000e-06	0.00591	1.029	2.012
elt_000_10885	Ga ₂ Nd ₃ Pd	6	-4.453	-4.775	1.000e-06	0.00449	1.29	1.465
elt_000_10902	Ge ₂ ReTb ₄	7	-5.783	-6.064	-3.000e-06	0.00971	0.83	0.981
elt_000_10921	Cd ₃ Fe ₂ YYb ₂	8	-3.361	-3.505	-5.000e-05	0.00669	0.266	0.894
elt_000_10930	As ₃ CdNi ₂	6	-3.568	-4.306	1.000e-06	0.00742	0.812	1.135
elt_000_10945	AuDy ₂ GaPd ₂ Sn	7	-4.737	-4.99	-9.000e-06	0.00528	0.632	0.84
elt_000_10954	Ga ₂ NdPdTb ₂	6	-4.473	-4.744	-1.500e-05	0.00693	0.987	1.043
elt_000_10960	CoGa ₂ GeNi ₂	6	-4.544	-4.805	-5.000e-06	0.00905	0.257	0.398
elt_000_10973	Nd ₂ NiTe ₄ Tl	8	-4.437	-4.574	-1.000e-06	0.00503	0.481	0.587
elt_000_11001	Dy ₂ GaPdSnSr ₃	8	-3.198	-3.51	1.000e-06	0.00313	1.055	1.402
elt_000_11012	CdNd ₃ Si ₄	8	-4.74	-4.952	-1.000e-06	0.00576	0.553	0.565
elt_000_11021	AuHfRu ₂ Si	5	-7.175	-7.736	1.000e-06	0.00582	0.411	0.499
elt_000_11068	Ge ₃ Tb ₃	6	-4.835	-5.28	-7.000e-06	0.00702	0.642	1.006
elt_000_11097	Ga ₃ Tb ₃	6	-3.909	-4.241	0.000e+00	0.0055	1.04	1.51
elt_000_11119	AlGd ₂ Ge ₂ Y	6	-4.99	-5.282	-1.000e-06	0.00547	0.595	1.681
elt_000_11123	Nd ₃ Zn ₄	7	-2.786	-2.876	-1.000e-06	0.00371	0.864	1.024
elt_000_11136	FeRu ₂ Se ₄	7	-4.972	-5.989	0.000e+00	0.0096	0.545	0.453
elt_000_11154	AuDy ₃ Sn ₂	6	-4.454	-4.747	-1.000e-06	0.00992	0.777	1.062
elt_000_11165	Gd ₃ GeSi ₂ Zn	7	-4.33	-4.694	0.000e+00	0.00525	0.719	0.92
elt_000_11172	Ru ₂ SnZn ₃	6	-3.9	-4.157	1.000e-06	0.00932	0.413	0.337
elt_000_11188	BrCuNd ₂ OsS	6	-4.984	-5.696	-1.900e-05	0.00565	1.897	2.512
elt_000_11189	AsNd ₂ Pt ₂ Yb	6	-5.221	-5.704	-3.000e-06	0.00678	0.868	1.912
elt_000_11195	Dy ₂ Ga ₃ Sn	6	-3.623	-4.114	2.000e-06	0.00779	1.154	1.715
elt_000_11232	Ga ₃ Tb ₃	6	-3.92	-4.241	2.000e-06	0.00909	0.84	0.975
elt_000_11234	Dy ₂ Gd ₂ Pt ₃ Sb	8	-5.719	-5.98	2.000e-06	0.00857	0.743	1.002
elt_000_11242	AsCeCo ₂ FeSn	6	-5.798	-6.267	-1.200e-05	0.0075	0.993	2.371
elt_000_11244	BaDy ₂ Pd ₂	5	-4.436	-4.847	-8.000e-06	0.00284	1.34	2.55
elt_000_11250	Ga ₃ Nd ₂ Sr	6	-3.418	-3.713	0.000e+00	0.00627	0.936	1.077

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_11283	AuGe ₂ Ru ₂	5	-4.992	-6.035	-2.700e-05	0.00581	0.421	0.837
elt_000_11293	Cu ₂ SbScTb ₂	6	-4.625	-4.81	-6.000e-06	0.00506	0.411	0.586
elt_000_11299	As ₂ NiTb ₃	6	-5.023	-5.649	-1.100e-05	0.00907	1.568	2.866
elt_000_11318	LaNd ₂ Zn ₃	6	-2.962	-3.164	1.000e-06	0.00469	1.095	0.966
elt_000_11341	Au ₂ LaRu ₂ Si	6	-5.582	-6.024	-4.000e-06	0.00373	0.773	1.013
elt_000_11346	AlCu ₃ Mn ₂	6	-5.167	-5.383	6.000e-06	0.00937	0.799	0.952
elt_000_11364	Co ₃ CrSbV	6	-6.839	-7.045	1.000e-06	0.00584	0.215	0.295
elt_000_11432	Gd ₂ NaSnZn ₂	6	-2.642	-3.034	-1.100e-05	0.00482	1.034	2.333
elt_000_11444	Nd ₃ S ₄ V	8	-6.111	-6.298	-4.000e-06	0.00409	0.411	0.602
elt_000_11446	AsAu ₂ Co ₂ Ge	6	-4.349	-4.89	-1.000e-06	0.00645	0.903	1.021
elt_000_11459	Au ₂ Gd ₂ RbSb ₂	7	-3.846	-4.099	-6.000e-06	0.0037	0.792	1.069
elt_000_11465	GaNi ₃ SmSnYb ₂	8	-3.863	-4.205	-1.000e-06	0.0052	0.887	1.615
elt_000_11476	CdNd ₂ Sb	4	-3.559	-4.175	-3.000e-06	0.00712	1.117	1.079
elt_000_11494	Ge ₂ NiPTb ₃ Zn	8	-4.381	-4.902	1.000e-06	0.00813	1.518	1.863
elt_000_11500	GeMn ₃ MoOs	6	-8.585	-8.784	-2.200e-05	0.0099	0.304	0.799
elt_000_11526	Se ₄ Tb ₂	6	-4.883	-5.409	1.000e-06	0.00376	0.91	0.996
elt_000_11558	CdNd ₂ Pr	4	-3.464	-3.823	-1.000e-06	0.00456	1.028	2.352
elt_000_11562	AlGaHf ₂ Ru ₂	6	-7.458	-7.836	0.000e+00	0.00722	0.528	0.506
elt_000_11564	Ag ₂ GeNd ₂ Te ₂	7	-3.857	-4.261	-3.000e-06	0.00404	1.123	1.582
elt_000_11620	Si ₄ SrYb ₂	7	-3.765	-3.961	-2.000e-06	0.00551	0.967	0.892
elt_000_11633	DyGa ₄ Gd ₂	7	-3.8	-4.031	1.000e-06	0.00493	0.671	0.856
elt_000_11645	AuCaCu ₂ Tb ₂	6	-3.626	-3.971	-6.000e-06	0.00288	0.655	1.795
elt_000_11647	CeGa ₃ Yb ₂	6	-3.045	-3.337	-3.200e-05	0.00519	1.188	1.121
elt_000_11656	Cd ₂ Nd ₂ RbSb ₃	8	-3.232	-3.518	0.0000e+00	0.00414	0.669	1.803
elt_000_11681	CBiDy ₂ Si ₄	8	-5.187	-5.559	-1.000e-06	0.0082	1.06	1.074
elt_000_11682	Al ₃ GeYb ₃	7	-2.799	-3.11	-5.000e-06	0.00537	0.655	1.971
elt_000_11683	CdGa ₂ Yb ₃	6	-2.005	-2.178	1.000e-06	0.0045	0.381	0.671
elt_000_11728	Au ₃ PrRu ₂	6	-5.112	-5.338	0.0000e+00	0.00969	0.228	0.367
elt_000_11753	Al ₂ Fe ₃ Nb	6	-6.94	-7.073	0.0000e+00	0.00455	0.214	0.275
elt_000_11771	CaAl ₂ Dy ₃ Si	7	-5.058	-5.294	1.000e-06	0.00506	0.685	0.913
elt_000_11786	Cd ₃ Nd ₂ Pt ₂ Sn	8	-3.708	-4.064	-2.000e-06	0.00488	1.579	2.311
elt_000_11805	Mn ₂ Si ₂ Sn ₂	6	-5.161	-5.95	0.0000e+00	0.00507	0.667	0.661
elt_000_11829	Co ₄ FeNi	6	-6.626	-6.729	-1.000e-06	0.00674	0.225	0.217
elt_000_11832	AsBRu ₂ SnVW	7	-7.691	-7.911	5.000e-06	0.00963	0.292	0.323
elt_000_11840	CuDy ₃ Ga ₂	6	-3.983	-4.282	-1.500e-05	0.00562	0.969	1.023
elt_000_11875	AlNd ₂ SiTe ₄	8	-4.417	-4.578	0.0000e+00	0.00924	0.333	0.394
elt_000_11896	Ru ₂ W ₆	8	-11.216	-11.684	-4.000e-06	0.00569	0.519	0.422
elt_000_11952	Al ₂ PdPtTb ₃ Ti	8	-5.319	-5.532	-1.157e-03	0.0087	0.391	1.145
elt_000_11976	Sb ₃ Tb ₃	6	-4.734	-5.287	-2.000e-06	0.00305	0.566	1.891
elt_000_12005	FeGaMn ₂ Sb ₂	6	-5.348	-5.965	0.0000e+00	0.00529	0.643	1.135
elt_000_12006	Dy ₄ Ga ₄	8	-3.667	-4.272	-1.000e-06	0.00521	0.809	0.775
elt_000_12042	CoGd ₄ RhSnZn	8	-4.812	-5.034	-1.000e-06	0.00591	1.084	2.189
elt_000_12043	AgAl ₃ KNiTb ₂	8	-3.623	-3.796	-1.300e-05	0.00533	0.644	0.742
elt_000_12070	Al ₂ Nd ₃ Pt	6	-4.796	-5.219	-1.000e-06	0.00416	1.729	1.985
elt_000_12081	GaSn ₂ Yb ₄ Zn	8	-2.393	-2.575	-3.000e-06	0.00635	1.064	1.377
elt_000_12086	AuDy ₃ GaZn	6	-3.631	-3.952	-7.000e-06	0.00684	0.675	0.758
elt_000_12088	CdCsDy ₂ GeRbSbTe	8	-3.249	-3.433	0.0000e+00	0.00273	0.891	1.22
elt_000_12090	Ge ₂ MoPtSeTb ₂ Zn	8	-5.177	-5.439	-1.000e-06	0.00583	0.703	1.144
elt_000_12100	MgNd ₂ Sb ₄	7	-4.019	-4.516	-1.300e-05	0.00784	2.008	2.724
elt_000_12111	BaCd ₂ Gd ₂ Sb	6	-2.718	-3.163	-2.000e-06	0.00408	0.715	1.639
elt_000_12112	CeFe ₄ Ga	6	-6.47	-6.801	-1.000e-06	0.00424	0.328	0.32
elt_000_12116	GaMgSbYYb ₂	6	-3.18	-3.345	-4.000e-06	0.00511	1.007	1.305

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_12118	Dy ₃ Ni ₂ Sn	6	-5.027	-5.249	-4.900e-05	0.00479	1.032	1.649
elt_000_12127	InPbTlYb ₂	5	-2.562	-2.619	-2.000e-06	0.00343	0.809	1.165
elt_000_12147	Gd ₃ IOs ₂	6	-5.993	-6.45	-2.000e-06	0.00801	0.954	2.278
elt_000_12178	Pd ₂ SnYb ₃	6	-3.569	-3.896	-5.000e-06	0.00279	1.088	3.768
elt_000_12189	Ru ₂ Sb ₄ Ti	7	-5.419	-6.234	2.000e-06	0.00569	1.05	1.498
elt_000_12196	GaGd ₂ Sn ₂ Sr	6	-3.724	-4.03	0.000e+00	0.00421	1.046	1.188
elt_000_12205	Cu ₂ GaN ₂ Sr	6	-3.457	-3.766	1.000e-06	0.00347	0.621	0.782
elt_000_12217	AgHgSnTe ₃ Yb ₂	8	-2.783	-3.02	0.000e+00	0.00768	0.973	1.348
elt_000_12223	CaGa ₃ Gd ₂	6	-3.415	-3.764	-1.000e-06	0.00391	1.02	1.284
elt_000_12234	CoGaNd ₃ Ni ₂ Pt	8	-5.103	-5.535	-6.000e-06	0.00666	0.67	1.037
elt_000_12266	Dy ₃ RhSb ₂	6	-4.942	-5.643	0.000e+00	0.00588	0.906	2.103
elt_000_12300	As ₂ Fe ₂ P ₂	6	-5.406	-6.123	-1.000e-06	0.00679	0.623	0.58
elt_000_12334	Mn ₂ MoSn ₃	6	-5.738	-6.519	-2.000e-06	0.00649	0.986	0.972
elt_000_12339	Cu ₂ Nd ₂ PrSb	6	-4.377	-4.697	-7.000e-06	0.00487	0.857	1.176
elt_000_12344	AlCoNd ₂ Zn ₃	7	-3.5	-3.644	0.000e+00	0.00892	0.651	1.651
elt_000_12357	AlAs ₂ GeNi ₂	6	-4.309	-4.845	-7.000e-06	0.00864	0.948	1.087
elt_000_12379	Dy ₂ PdSn ₂ W	6	-5.774	-6.077	-6.000e-06	0.00511	0.888	0.953
elt_000_12382	ErGa ₂ Gd ₂ Pt	6	-4.573	-4.99	0.000e+00	0.00951	1.149	2.393
elt_000_12402	GaPdTb ₃	5	-4.659	-4.756	-2.000e-06	0.00645	0.451	0.577
elt_000_12410	B ₃ GeOsRu ₂	7	-7.372	-7.603	2.000e-06	0.00571	0.324	0.433
elt_000_12429	ClNbNd ₂ Se ₂ Te	7	-5.324	-5.737	-2.000e-06	0.00437	1.033	1.083
elt_000_12431	Ga ₃ SrTb ₂	6	-3.388	-3.651	-1.000e-06	0.0043	0.955	0.916
elt_000_12456	Cu ₂ Dy ₃ Ni	6	-4.272	-4.667	-1.350e-04	0.0075	0.637	1.957
elt_000_12457	CeRu ₂ SiTiV ₂	7	-6.904	-7.167	1.000e-06	0.00473	0.959	1.408
elt_000_12492	Fe ₃ Si ₂ Sn	6	-5.928	-6.389	-2.000e-06	0.00946	0.448	0.482
elt_000_12493	DyRhTb ₂ Zn	5	-4.497	-4.734	0.000e+00	0.0034	0.298	1.729
elt_000_12505	CeGd ₂ Rh ₄ Si	8	-6.321	-6.984	0.000e+00	0.00411	1.352	1.505
elt_000_12531	Mn ₂ PdSn ₃	6	-4.62	-5.61	-2.000e-06	0.00429	0.873	2.367
elt_000_12537	Dy ₂ Sb ₂ Te	5	-4.326	-5.0	0.000e+00	0.00402	1.553	3.23
elt_000_12560	Dy ₃ Pt ₂ Si	6	-5.798	-6.152	3.000e-06	0.00482	0.516	0.681
elt_000_12568	Si ₃ Tb ₃	6	-5.157	-5.551	0.000e+00	0.0058	0.513	0.742
elt_000_12577	Gd ₂ OsSn ₄	7	-5.047	-5.4	0.000e+00	0.00614	0.88	1.441
elt_000_12590	Dy ₃ GaRh	5	-4.9	-5.306	0.000e+00	0.00885	1.029	2.311
elt_000_12612	Fe ₂ PSbSr	5	-4.562	-5.668	7.000e-06	0.00576	1.255	1.946
elt_000_12617	Li ₂ Ni ₂ O ₂	6	-4.795	-5.114	-4.000e-06	0.00497	0.787	0.909
elt_000_12622	AuReYb ₄	6	-3.445	-3.613	-1.000e-05	0.00902	0.935	1.263
elt_000_12644	BaCd ₂ Dy ₂ MgSb	7	-2.72	-2.857	0.000e+00	0.00351	0.489	0.682
elt_000_12653	GaGd ₃ Si	5	-4.493	-4.783	0.000e+00	0.0088	0.547	0.578
elt_000_12661	Br ₄ CuTb ₃	8	-3.682	-4.16	-4.000e-06	0.00453	0.708	1.026
elt_000_12663	As ₃ Nd ₃	6	-5.253	-6.202	-1.000e-06	0.00189	1.135	1.614
elt_000_12664	AsDy ₂ Pt ₂ Si ₃	8	-5.601	-6.071	-1.000e-06	0.00505	0.958	1.331
elt_000_12665	BaPbPdTb ₂	5	-4.124	-4.327	-1.000e-06	0.00616	0.933	1.065
elt_000_12686	Sn ₆ Yb ₂	8	-3.319	-3.471	1.000e-06	0.00584	0.567	0.74
elt_000_12696	PbSbTb ₂	4	-4.159	-4.886	0.000e+00	0.00634	1.554	1.956
elt_000_12702	Ga ₃ Mn ₂ Sb	6	-4.673	-4.954	0.000e+00	0.00978	0.38	0.39
elt_000_12708	Al ₄ Nd ₂ Pr	7	-4.059	-4.263	-2.000e-06	0.00295	0.32	0.854
elt_000_12711	Dy ₃ Ga ₃	6	-3.865	-4.229	1.000e-06	0.00806	0.854	1.886
elt_000_12763	Ga ₃ Tb ₃	6	-3.943	-4.241	-9.000e-06	0.00817	0.902	2.021
elt_000_12776	Au ₂ CaDy ₂ Sb	6	-4.089	-4.355	-2.000e-06	0.00432	0.608	0.723
elt_000_12788	Co ₂ NbSe ₃	6	-4.753	-5.857	2.000e-06	0.00944	0.823	2.032
elt_000_12809	Dy ₃ Ga ₂	5	-3.848	-4.333	-1.000e-06	0.00658	1.61	1.574
elt_000_12826	AlGa ₂ Tb ₃	6	-3.865	-4.305	1.000e-06	0.00585	1.049	1.186

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_12837	AuGe ₂ Mn ₃	6	-5.911	-6.361	-8.000e-06	0.00913	0.644	1.979
elt_000_12842	As ₃ Dy ₃ Ni	7	-5.337	-5.691	1.000e-06	0.00634	1.476	1.892
elt_000_12854	Ru ₂ Zr ₄	6	-8.664	-9.101	-1.000e-06	0.00839	0.504	1.349
elt_000_12860	InPd ₂ Yb ₃	6	-3.669	-3.621	-6.000e-06	0.00385	0.731	0.782
elt_000_12862	As ₄ CoDy ₂ Ta	8	-6.165	-6.411	-7.000e-06	0.00712	0.428	0.593
elt_000_12874	As ₂ Dy ₂ MoPSi	7	-5.764	-6.254	-1.000e-06	0.00655	1.08	0.996
elt_000_12898	Co ₃ MoSe ₂	6	-5.714	-6.299	-7.000e-06	0.00904	0.668	0.783
elt_000_12899	AsCo ₃ Sb ₂	6	-4.364	-5.5	-3.000e-06	0.00582	0.77	0.892
elt_000_12932	Al ₂ AuNd ₃	6	-4.194	-4.588	-1.000e-06	0.00241	1.223	2.224
elt_000_12937	Ga ₃ Nd ₃	6	-4.011	-4.291	-3.000e-06	0.00516	0.838	0.858
elt_000_12943	Gd ₂ NiSbSn ₂	6	-4.603	-5.034	-1.700e-04	0.00804	0.85	1.315
elt_000_12950	Co ₂ Dy ₂ GaNd	6	-5.02	-5.315	-2.000e-06	0.00572	0.972	0.814
elt_000_12963	Pt ₄ TeYb ₃	8	-4.494	-4.71	6.000e-06	0.00775	0.409	0.427
elt_000_12971	AgGd ₂ Mg ₂ Pt ₃	8	-4.479	-4.698	0.000e+00	0.00397	0.6	0.817
elt_000_12991	Ni ₃ Sb ₃	6	-4.427	-4.76	-9.300e-05	0.00925	0.498	0.58
elt_000_12997	Gd ₂ Rb ₂ Te ₂	6	-3.421	-3.568	-1.100e-05	0.00314	0.907	0.996
elt_000_13006	Fe ₂ Ga ₃ Ti	6	-5.3	-5.574	-3.000e-06	0.00379	0.454	0.517
elt_000_13010	Ru ₂ Si ₃ Sr	6	-5.986	-6.281	1.000e-06	0.00574	0.309	0.315
elt_000_13032	CoFePSi ₂ Tb ₂	7	-6.073	-6.45	0.000e+00	0.00733	0.705	1.844
elt_000_13053	Nd ₂ Pt ₆	8	-5.857	-6.582	0.000e+00	0.00736	1.013	2.003
elt_000_13107	GeRu ₃ Sb ₃	7	-5.763	-6.334	-5.000e-06	0.00654	0.674	0.538
elt_000_13115	As ₄ Fe ₂	6	-4.655	-5.928	-5.000e-06	0.00499	0.739	0.87
elt_000_13126	Hf ₄ Ru ₂	6	-9.368	-9.992	-2.600e-05	0.0067	0.339	0.385
elt_000_13153	Au ₂ Dy ₄ Zn ₂	8	-3.825	-3.946	-4.000e-06	0.00319	0.362	0.788
elt_000_13177	As ₃ Mn ₂ V	6	-6.197	-6.862	-1.000e-06	0.00551	0.459	0.436
elt_000_13187	GaLuRu ₂ Sb ₂	6	-5.525	-6.003	-2.000e-06	0.00873	0.714	0.865
elt_000_13217	AlGd ₃ Pt ₄	8	-5.942	-6.149	2.000e-06	0.0057	0.342	0.915
elt_000_13219	Fe ₃ PRh ₂	6	-7.2	-7.481	-8.000e-06	0.00786	0.214	0.339
elt_000_13221	Al ₂ GaLiRu ₂	6	-5.104	-5.272	0.000e+00	0.00822	0.357	1.242
elt_000_13230	Cd ₂ Pb ₂ Yb ₃	7	-2.079	-2.236	-1.000e-06	0.00424	1.511	2.467
elt_000_13242	Cl ₄ Gd ₂	6	-4.502	-4.678	-5.000e-06	0.00507	0.633	0.647
elt_000_13284	Gd ₃ Ni ₂ Sb	6	-5.15	-5.37	-7.000e-06	0.00745	0.738	0.913
elt_000_13286	Gd ₂ Pt ₃ Sn	6	-5.772	-6.087	0.000e+00	0.00654	1.077	1.256
elt_000_13300	Al ₂ Er ₂ Ga ₂ Tb ₂	8	-3.643	-4.312	0.000e+00	0.00611	0.719	1.029
elt_000_13314	Ga ₃ LaTb ₂	6	-3.957	-4.292	-1.000e-06	0.00891	0.95	0.971
elt_000_13322	Al ₂ GeSiTb ₃	7	-4.432	-4.712	-2.000e-06	0.00535	0.787	2.081
elt_000_13326	As ₃ Gd ₂ Te	6	-4.588	-5.271	0.000e+00	0.00295	1.55	2.262
elt_000_13335	Pt ₂ SbTb ₄ Ti	8	-5.833	-6.125	-5.000e-06	0.00463	1.667	2.618
elt_000_13343	AsGe ₃ Ni ₂	6	-4.095	-4.837	-3.000e-06	0.00996	0.694	0.629
elt_000_13350	Nd ₂ Ni ₂ Sn ₃	7	-4.607	-4.856	3.000e-06	0.0048	0.908	2.328
elt_000_13358	Al ₃ Gd ₃	6	-4.159	-4.508	0.000e+00	0.00327	1.116	1.128
elt_000_13372	AgGa ₂ Nd ₂ Sn	6	-3.768	-4.041	-1.000e-06	0.00726	1.542	1.455
elt_000_13384	Dy ₂ EuSn	4	-3.7	-4.047	-1.000e-06	0.00967	0.829	0.928
elt_000_13392	CoFe ₂ MoSn ₂	6	-5.907	-6.662	-4.000e-06	0.0099	0.638	0.582
elt_000_13394	As ₂ Fe ₂ SbTi	6	-5.351	-6.343	-1.000e-06	0.00467	0.544	0.625
elt_000_13396	Dy ₃ GaRhSi ₂	7	-5.373	-5.629	0.000e+00	0.0053	0.888	0.967
elt_000_13415	AgCu ₂ Dy ₃	6	-3.958	-4.163	-4.000e-06	0.00908	0.447	0.573
elt_000_13443	SrTlYb ₃ Zn	6	-1.61	-1.766	0.000e+00	0.00433	0.76	3.054
elt_000_13458	Gd ₂ SnSr ₃	6	-2.878	-3.075	-7.000e-06	0.00521	0.48	0.5
elt_000_13474	GePtRu ₂ ScSi	6	-6.892	-7.223	-1.000e-06	0.00505	0.765	0.977
elt_000_13485	AuMgRu ₂ SnZn	6	-4.239	-4.647	0.000e+00	0.00564	0.421	0.454
elt_000_13493	Ga ₂ Nd ₃ Pt	6	-4.611	-4.974	-3.000e-06	0.00491	1.203	1.446

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_13496	Ga ₂ Ge ₂ Ru ₂ Sn	7	-4.833	-5.297	1.000e-06	0.00817	0.757	1.544
elt_000_13502	C ₂ Na ₂ Tb ₂	6	-4.058	-4.736	0.000e+00	0.00894	1.735	1.702
elt_000_13507	Ga ₂ LiRu ₃	6	-5.743	-5.887	-7.000e-06	0.00821	0.266	0.291
elt_000_13509	Br ₄ Dy ₂ O	7	-4.774	-5.203	-4.000e-06	0.00883	0.536	0.796
elt_000_13521	CdGa ₂ Yb ₃	6	-2.032	-2.219	-1.000e-06	0.00469	0.956	1.171
elt_000_13523	Nd ₂ NiSn ₂ Sr	6	-4.059	-4.527	1.000e-06	0.00418	1.706	2.136
elt_000_13536	Gd ₂ Ge ₃ Sm	6	-4.858	-5.2	2.000e-06	0.00803	0.487	0.732
elt_000_13549	Dy ₂ La ₂ RhSi ₃	8	-5.524	-5.875	-1.000e-06	0.00474	0.675	0.886
elt_000_13551	AsFeMgNd ₂ RhTl	7	-4.867	-5.109	-1.000e-05	0.00733	0.631	0.766
elt_000_13558	Br ₄ Mn ₂	6	-3.726	-4.218	-3.000e-06	0.00735	1.046	1.641
elt_000_13562	Al ₄ Dy ₂ Sn	7	-4.004	-4.375	-1.000e-06	0.00364	0.846	0.987
elt_000_13568	AuCdSb ₃ Tb ₂	7	-3.898	-4.212	0.000e+00	0.00598	1.341	3.077
elt_000_13578	Gd ₃ Sb ₂ Sn	6	-4.445	-5.15	-3.000e-06	0.00652	0.649	1.255
elt_000_13600	Dy ₂ Fe ₂ SnTe	6	-5.303	-5.766	-5.000e-06	0.00708	1.166	0.813
elt_000_13624	P ₃ Ru ₂ W	6	-7.703	-8.036	0.000e+00	0.00573	0.418	0.547
elt_000_13625	Ga ₃ Gd ₂ Sm	6	-3.964	-4.26	-1.000e-06	0.00591	0.874	0.793
elt_000_13640	CdGd ₃ Mg ₂ Sb	7	-3.15	-3.256	1.000e-06	0.00361	0.419	0.451
elt_000_13651	BaNd ₂ Sb	4	-3.864	-4.226	2.000e-06	0.00597	1.689	1.4
elt_000_13690	AlGaNd ₄	6	-4.366	-4.543	0.000e+00	0.0028	1.258	1.328
elt_000_13704	GeRu ₃ Zr ₃	7	-8.246	-8.593	-2.000e-06	0.00565	0.836	1.393
elt_000_13705	CaCd ₂ Dy ₂ Si ₂	7	-3.41	-3.583	0.000e+00	0.00289	0.638	0.846
elt_000_13710	I ₄ Tb ₂	6	-3.65	-3.695	-1.000e-06	0.0067	0.243	0.159
elt_000_13725	AlGa ₂ Nd ₃	6	-4.081	-4.376	2.000e-06	0.00858	0.894	0.943
elt_000_13733	BaSb ₂ Yb ₂	5	-2.869	-3.432	1.000e-06	0.00529	1.25	1.865
elt_000_13734	CdGd ₃ Pd ₂	6	-4.461	-4.798	-1.000e-06	0.00368	0.947	1.178
elt_000_13735	Ru ₃ Si ₃ Yb	7	-6.876	-7.027	-1.600e-05	0.00584	0.289	0.32
elt_000_13764	Nd ₂ RbSb	4	-3.441	-3.736	-8.000e-06	0.00482	1.489	1.763
elt_000_13768	As ₂ AuDy ₂ Y	6	-5.002	-5.794	-1.000e-06	0.00367	0.731	1.117
elt_000_13780	CrSn ₅ Yb ₂	8	-3.736	-4.068	8.000e-06	0.00641	0.326	0.579
elt_000_13813	As ₃ AuNd ₂ Sr	7	-4.477	-5.172	0.000e+00	0.00327	1.303	2.2
elt_000_13816	Al ₂ Gd ₃ Sb	6	-4.437	-4.689	-1.000e-06	0.00374	0.746	0.789
elt_000_13824	Gd ₃ SbSrZn ₃	8	-2.806	-3.159	3.000e-06	0.00664	1.13	1.196
elt_000_13842	As ₂ Fe ₃ Si	6	-6.182	-6.438	-2.000e-06	0.00992	0.321	0.44
elt_000_13847	Ga ₂ Gd ₂ NiV ₃	8	-5.548	-6.078	-5.000e-06	0.00483	1.199	1.485
elt_000_13859	CoDy ₆ Mn	8	-5.208	-5.398	-3.000e-06	0.0067	0.489	0.659
elt_000_13879	BaBiYb ₂	4	-2.326	-2.638	0.000e+00	0.00348	1.011	2.564
elt_000_13886	AuGa ₃ Gd ₂	6	-3.839	-4.162	-2.200e-05	0.00667	1.209	1.461
elt_000_13906	AlSn ₃ Tb ₃	7	-4.191	-4.499	-6.000e-06	0.00819	1.346	1.468
elt_000_13909	Ge ₂ Ni ₃ Sn	6	-4.314	-4.916	-1.000e-06	0.00682	0.914	1.145
elt_000_13933	Ga ₃ SrTb ₂	6	-3.355	-3.65	-5.000e-05	0.00702	0.876	1.017
elt_000_13943	AlCo ₅ Tb ₂	8	-5.569	-5.945	-7.000e-06	0.00852	1.032	1.52
elt_000_13952	Au ₂ Gd ₃ Mg	6	-3.905	-4.073	2.000e-06	0.00225	0.495	0.423
elt_000_13953	AgAu ₂ Tb ₃	6	-4.043	-4.51	0.000e+00	0.00371	1.333	2.166
elt_000_13961	AuGe ₂ Nd ₂ Sm	6	-4.729	-5.101	-1.000e-06	0.00662	0.752	0.978
elt_000_14024	Au ₂ Ru ₂	4	-5.399	-5.82	-1.000e-06	0.0034	0.308	1.715
elt_000_14027	SnTb ₃ Zn ₂	6	-3.36	-3.645	1.000e-06	0.00459	1.087	1.028
elt_000_14066	Al ₂ GdRu ₂ Si	6	-6.03	-6.33	1.000e-06	0.00759	0.404	0.284
elt_000_14075	MoNd ₃ Sn ₃	7	-5.143	-5.378	-2.000e-06	0.00667	0.503	0.988
elt_000_14077	Ga ₃ SmTb ₂	6	-3.958	-4.254	0.000e+00	0.00567	0.888	1.888
elt_000_14088	Fe ₂ GaY	4	-5.569	-6.359	-2.000e-06	0.00708	0.562	0.785
elt_000_14099	Nd ₃ Si ₃	6	-5.243	-5.609	0.000e+00	0.00518	1.078	1.219
elt_000_14113	GeLa ₂ Sb ₂ SiYb ₂	8	-4.08	-4.525	-5.000e-06	0.00843	1.511	3.175

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_14118	Gd ₂ SnSrTe ₂	6	-4.065	-4.692	-1.100e-05	0.0052	1.19	1.636
elt_000_14122	Ga ₂ Gd ₂ PrSb	6	-4.136	-4.56	-1.000e-06	0.0043	0.994	1.141
elt_000_14129	Nd ₃ PdSb ₃	7	-4.801	-5.34	-7.000e-06	0.00447	0.916	1.715
elt_000_14131	AsGa ₂ PrRu ₂	6	-5.71	-5.917	0.000e+00	0.00314	0.626	0.726
elt_000_14133	Ga ₂ PdSbYb ₃	7	-3.178	-3.381	0.000e+00	0.00624	0.553	0.409
elt_000_14140	AsGd ₂ GeSnW ₃	8	-6.999	-7.57	0.000e+00	0.00882	0.406	0.374
elt_000_14166	GaNd ₂ PdSr	5	-4.053	-4.213	-1.200e-05	0.00501	1.517	1.859
elt_000_14168	Dy ₃ Pd ₃	6	-5.328	-5.702	0.000e+00	0.00458	0.626	0.914
elt_000_14172	LaMgNd ₃ Pt ₃	8	-5.625	-5.711	0.000e+00	0.00606	0.256	0.305
elt_000_14173	Ga ₃ Gd ₃	6	-3.952	-4.257	0.000e+00	0.00685	0.966	0.734
elt_000_14179	Dy ₃ MgRh ₂ SiSn	8	-5.348	-5.467	-4.100e-05	0.00572	0.555	0.709
elt_000_14204	AuRu ₂ SbSiZr	6	-6.337	-6.826	0.000e+00	0.00777	0.307	0.406
elt_000_14242	Dy ₂ NiSn ₄	7	-4.474	-4.611	1.000e-06	0.00531	0.727	0.885
elt_000_14248	Gd ₃ Pt ₄ Zn	8	-5.468	-5.826	-1.000e-06	0.00491	0.559	0.64
elt_000_14263	Al ₄ Gd ₂ Sb	7	-4.037	-4.467	-9.000e-06	0.00344	1.061	1.251
elt_000_14265	Dy ₃ GaNi ₂	6	-4.768	-5.03	3.000e-06	0.00827	0.873	1.06
elt_000_14271	Fe ₃ Ge ₂ Sb	6	-5.56	-6.066	-1.100e-05	0.00783	0.505	0.669
elt_000_14291	BaSn ₄ Yb ₂	7	-3.145	-3.33	-2.300e-05	0.00889	0.861	1.073
elt_000_14313	Ga ₃ Tb ₂ Yb	6	-3.331	-3.698	0.000e+00	0.00837	0.835	0.934
elt_000_14320	Cd ₂ Dy ₃ Pd	6	-3.428	-3.893	-1.000e-06	0.00676	1.136	1.674
elt_000_14331	Ge ₄ Mn ₂	6	-5.533	-5.899	-1.000e-05	0.00749	0.908	0.983
elt_000_14332	HgMgTlYb ₃	6	-1.486	-1.651	-4.000e-06	0.00568	1.161	1.129
elt_000_14348	GaSe ₄ Yb ₃	8	-3.985	-4.239	-1.000e-06	0.00617	0.825	0.663
elt_000_14354	Gd ₃ Rh ₂ Si ₂ Zr	8	-6.567	-6.742	-1.100e-05	0.00541	0.441	0.565
elt_000_14389	Co ₂ Ga ₂ Ge ₂	6	-4.47	-4.96	-4.400e-05	0.00703	0.577	0.764
elt_000_14390	Dy ₃ Ga ₃	6	-3.857	-4.226	0.000e+00	0.00627	0.822	0.955
elt_000_14436	Ga ₃ Nd ₃	6	-3.986	-4.29	0.000e+00	0.0049	1.066	2.069
elt_000_14438	LaNi ₂ PdSnTb ₂	7	-4.893	-5.357	-2.100e-05	0.00559	1.295	3.778
elt_000_14465	As ₃ Co ₃	6	-5.122	-5.795	3.000e-06	0.00492	0.641	0.88
elt_000_14488	Sn ₃ Tb ₂	5	-4.135	-4.642	0.000e+00	0.00376	1.064	1.13
elt_000_14489	Co ₂ Ge ₂ ReY	6	-6.831	-7.054	-2.000e-06	0.00985	0.428	0.604
elt_000_14502	Cd ₆ Gd ₂	8	-1.592	-1.968	1.000e-06	0.00561	1.78	3.226
elt_000_14516	Gd ₃ Pt ₃ Y	7	-6.279	-6.496	0.000e+00	0.00568	0.28	0.524
elt_000_14527	AuGaMgNiTb ₂	6	-3.97	-4.073	-3.000e-06	0.00241	0.372	0.46
elt_000_14534	As ₂ Mn ₃ P ₂ Sn	8	-6.061	-6.446	-2.000e-06	0.00672	0.557	2.225
elt_000_14535	GeMn ₂ ScZn ₂	6	-4.687	-5.131	-1.000e-06	0.00789	0.967	1.06
elt_000_14541	Dy ₃ Ga ₃	6	-3.912	-4.227	0.000e+00	0.00619	0.836	1.039
elt_000_14569	Al ₂ AsPrRu ₂	6	-5.959	-6.2	-2.000e-06	0.00616	0.476	0.624
elt_000_14598	Dy ₂ Ge ₂ ISi ₃	8	-4.583	-4.839	1.000e-06	0.00755	0.659	1.699
elt_000_14600	AgGa ₂ Nd ₃	6	-3.909	-4.177	0.000e+00	0.00464	1.151	1.22
elt_000_14619	Ga ₃ Gd ₂ MgSr	7	-3.004	-3.397	-1.000e-06	0.00682	0.889	1.431
elt_000_14642	Nd ₂ OsSi ₂ Tm	6	-6.091	-6.35	-4.000e-06	0.00685	0.851	0.962
elt_000_14653	Cs ₂ HgSbTb ₂	6	-2.49	-2.731	3.000e-06	0.00697	0.988	1.074
elt_000_14670	IrSi ₃ Tb ₃	7	-5.924	-6.214	-1.000e-06	0.00651	0.556	0.76
elt_000_14678	AsCo ₄ Mo	6	-6.972	-7.108	-1.600e-05	0.00672	0.307	0.303
elt_000_14688	Fe ₂ Te ₄	6	-4.533	-4.731	2.000e-06	0.00845	0.444	1.455
elt_000_14696	Gd ₃ Pt ₂ Te ₂	7	-5.372	-5.657	-1.000e-06	0.00389	0.319	1.9
elt_000_14704	Ge ₄ Yb ₄	8	-3.43	-3.732	-1.200e-05	0.0085	0.618	0.715
elt_000_14710	CaGd ₃ OsP ₂	7	-5.984	-6.212	-3.000e-06	0.00272	0.315	0.45
elt_000_14715	Al ₂ EuGd ₂ Rh	6	-4.355	-4.748	3.000e-06	0.00647	1.082	1.569
elt_000_14723	CdNd ₃	4	-3.593	-3.863	-1.000e-06	0.00536	0.531	0.656
elt_000_14747	AuGaGd ₂ Ge ₂	6	-4.269	-4.717	-4.000e-06	0.00513	1.162	2.739

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_14787	Ge ₃ RhRu ₂ Si	7	-6.33	-6.462	1.000e-06	0.00996	0.367	0.434
elt_000_14788	Mn ₂ Si ₂ Sn ₃	7	-4.444	-5.643	0.000e+00	0.00528	0.742	1.721
elt_000_14808	K ₂ Rb ₂ Yb ₂	6	-0.667	-0.989	-1.470e-05	0.00444	1.807	1.892
elt_000_14828	Al ₃ Nd ₃	6	-4.18	-4.544	-7.000e-06	0.00444	1.284	1.705
elt_000_14830	AlGaSnTb ₂ Zn	6	-3.541	-3.921	1.000e-06	0.00596	1.405	2.058
elt_000_14833	AsDy ₃ Si ₃	7	-5.025	-5.704	0.000e+00	0.00561	1.367	2.165
elt_000_14838	Ga ₂ Ni ₃ Sb	6	-3.865	-4.526	-3.900e-05	0.0093	0.846	1.14
elt_000_14846	AsMn ₂ Se ₂ Te	6	-4.991	-5.605	0.000e+00	0.00541	0.623	0.618
elt_000_14850	Co ₂ Nd ₃ Sn ₂	7	-5.238	-5.469	-4.000e-06	0.00726	0.853	1.074
elt_000_14857	Ru ₂ Sc ₂ Si ₂	6	-7.164	-7.741	0.000e+00	0.00698	0.779	0.789
elt_000_14859	AlBLiRu ₂ S ₂ Sb	8	-5.48	-5.68	-2.000e-06	0.00964	0.974	1.653
elt_000_14876	AuSn ₂ Yb ₃	6	-2.898	-3.327	-2.000e-05	0.00754	1.461	1.835
elt_000_14891	Dy ₃ Ga ₂ Pd ₂	7	-4.825	-4.912	1.000e-06	0.00881	0.74	0.84
elt_000_14898	Ge ₃ Nd ₃	6	-4.825	-5.239	-1.000e-06	0.00829	0.945	1.116
elt_000_14902	Al ₄ Mn ₂	6	-5.366	-5.605	-5.000e-06	0.00583	0.229	0.25
elt_000_14907	Nd ₄ PdSmSn ₂	8	-4.806	-4.916	2.000e-06	0.00625	0.601	1.703
elt_000_14945	Ge ₂ Nd ₂ SnSr	6	-4.194	-4.6	1.000e-06	0.00599	0.58	0.853
elt_000_14977	Ge ₃ Nd ₃	6	-4.841	-5.24	-3.000e-06	0.00712	0.57	0.773
elt_000_14989	AlGeMgRu ₂ Tm	6	-5.459	-5.666	0.000e+00	0.00419	0.501	0.561
elt_000_14998	Co ₂ SiZn	4	-4.943	-5.335	-2.100e-05	0.00732	0.523	1.639
elt_000_14999	Al ₂ HfNi ₃	6	-5.831	-6.01	1.000e-06	0.00919	0.29	1.342
elt_000_15018	CMn ₂ Tb	4	-6.935	-7.886	-1.000e-06	0.00668	1.179	1.759
elt_000_15020	CuDy ₂ EuGa ₂	6	-3.308	-3.814	0.000e+00	0.00752	1.661	2.369
elt_000_15021	AlGd ₃ PtSb ₂	7	-4.692	-5.268	-1.000e-06	0.0069	0.875	3.189
elt_000_15023	Dy ₃ Ga ₂ Sb	6	-4.191	-4.549	-1.000e-06	0.0087	0.847	1.183
elt_000_15030	FeNi ₂ SbSn ₂ Te	7	-4.523	-4.843	-1.000e-06	0.00968	1.002	1.181
elt_000_15055	Cu ₃ Tb ₃	6	-4.057	-4.302	-1.340e-04	0.00567	0.74	1.004
elt_000_15108	Dy ₃ Ni ₂ Zn	6	-4.367	-4.573	1.000e-06	0.00659	0.223	0.48
elt_000_15114	Rh ₂ Ru ₂	4	-7.993	-8.233	-3.000e-06	0.00579	0.16	0.207
elt_000_15125	MgNaTb ₂ Zn ₂	6	-2.241	-2.384	-6.000e-06	0.00272	0.564	0.83
elt_000_15151	AlCa ₃ Nd ₂	6	-3.044	-3.147	-3.000e-06	0.00439	0.52	0.735
elt_000_15157	Co ₂ PV	4	-7.118	-7.321	-1.000e-06	0.00523	0.268	0.449
elt_000_15185	Cd ₂ LaNd ₂ RhSb	7	-3.932	-4.365	-1.000e-06	0.00617	0.451	0.694
elt_000_15218	Ga ₃ Gd ₃	6	-3.994	-4.256	-1.000e-06	0.00725	0.862	0.944
elt_000_15242	Hg ₃ Nd ₃	6	-2.549	-2.797	0.000e+00	0.00361	0.618	0.769
elt_000_15294	Dy ₃ Ga ₃	6	-3.953	-4.227	2.000e-06	0.00535	0.9	0.985
elt_000_15295	BiIr ₂ Yb ₅	8	-3.981	-4.073	0.000e+00	0.00526	0.351	0.886
elt_000_15333	P ₂ RuSnYb ₃	7	-4.464	-4.768	1.000e-06	0.00444	0.867	1.276
elt_000_15355	Mn ₂ P ₅	7	-5.67	-6.466	-7.000e-06	0.00644	0.584	0.561
elt_000_15357	CaNd ₂ Si ₂ Sn	6	-4.365	-4.823	-1.000e-06	0.00326	0.84	1.181
elt_000_15360	GeMn ₂ PtW ₂	6	-8.674	-9.037	-1.300e-05	0.00734	0.283	0.425
elt_000_15363	AuCaGa ₂ Nd ₂	6	-3.633	-3.885	0.000e+00	0.00553	1.025	1.213
elt_000_15377	CoGa ₄ Gd ₂	7	-4.263	-4.454	1.000e-06	0.00767	0.8	0.762
elt_000_15380	AlGe ₂ Nd ₃	6	-4.679	-5.07	-3.000e-06	0.00716	0.584	1.262
elt_000_15386	As ₃ BMo ₂ Ru ₂	8	-7.32	-7.679	0.000e+00	0.00739	0.176	0.471
elt_000_15387	Cu ₂ Gd ₃ SbSn	7	-4.514	-4.621	-7.000e-06	0.00345	0.957	1.179
elt_000_15391	Dy ₃ Si ₃	6	-5.093	-5.534	-2.000e-06	0.00396	0.484	0.604
elt_000_15428	Nd ₂ SeSnTe ₃	7	-4.406	-4.848	1.000e-06	0.00402	0.546	1.694
elt_000_15429	GaSbYb ₃ Zn	6	-2.322	-2.558	-1.000e-06	0.00327	1.136	1.554
elt_000_15467	AsCuNi ₃ P	6	-4.733	-5.125	-3.000e-06	0.00606	0.764	0.943
elt_000_15478	Gd ₂ MnNdNi ₂ Sn	7	-5.411	-5.582	-1.000e-06	0.00608	1.039	2.123
elt_000_15490	Ru ₃ Sn ₄	7	-5.641	-6.066	-1.000e-06	0.00523	0.49	0.584

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_15538	As ₂ MoNd ₂ Si ₂	7	-5.904	-6.3	0.000e+00	0.00332	0.514	1.664
elt_000_15551	Gd ₄ Rh ₂ Si ₂	8	-5.975	-6.271	-5.000e-06	0.00588	0.344	0.381
elt_000_15552	AlNd ₄ Pd ₂	7	-5.05	-5.244	0.000e+00	0.0072	0.489	1.719
elt_000_15553	Al ₃ Fe ₂ Zr	6	-5.928	-6.158	-9.000e-06	0.00838	0.268	0.317
elt_000_15563	Ag ₂ AlNd ₃	6	-3.83	-4.115	0.000e+00	0.00698	1.198	1.322
elt_000_15583	AgGa ₂ Tb ₃	6	-3.844	-4.115	-1.000e-06	0.00367	0.868	0.907
elt_000_15608	Ir ₂ LiNd ₃	6	-5.655	-6.083	-2.000e-06	0.00445	0.946	1.215
elt_000_15616	As ₂ AuGeNd ₂ RbSi	8	-4.019	-4.684	-1.000e-06	0.00372	0.417	1.576
elt_000_15617	Ga ₃ Nd ₃	6	-4.027	-4.291	-1.000e-06	0.00456	0.905	0.79
elt_000_15627	As ₄ Pt ₂ Ru ₂	8	-6.069	-6.277	1.000e-06	0.00692	0.747	0.829
elt_000_15651	CsNd ₂ SbTe ₃	7	-3.897	-4.445	-2.500e-05	0.00781	0.778	1.061
elt_000_15658	Al ₃ CoDy ₂ Sb ₂	8	-4.426	-4.542	-4.000e-06	0.0052	0.326	0.425
elt_000_15696	Co ₂ IrSm	4	-6.237	-6.824	2.000e-06	0.00859	1.25	2.562
elt_000_15704	Ga ₃ Ni ₃	6	-4.19	-4.367	-2.000e-06	0.00693	0.146	2.256
elt_000_15707	Gd ₂ Mn ₂ Se ₂	6	-4.714	-6.088	-1.300e-05	0.00768	0.772	0.622
elt_000_15717	Cd ₂ Gd ₂ Ti ₄	8	-4.898	-5.145	1.000e-06	0.00786	1.061	1.744
elt_000_15718	CaCuHg ₃ Yb ₂	7	-1.548	-1.624	1.000e-06	0.00692	1.266	1.32
elt_000_15734	AlFe ₂ Si ₂ Ti	6	-6.623	-6.775	0.000e+00	0.00647	0.126	1.198
elt_000_15756	BiNa ₂ Pd ₂ Tb ₂ Yb	8	-3.643	-3.812	-5.000e-06	0.00621	0.585	1.842
elt_000_15766	Dy ₂ GaTe ₃	6	-4.106	-4.512	-2.000e-06	0.00898	0.935	2.489
elt_000_15772	Pt ₄ Ru ₂	6	-6.46	-7.091	-1.000e-06	0.00848	0.397	0.478
elt_000_15773	Al ₂ Ga ₂ Nd ₃	7	-4.11	-4.23	-1.000e-06	0.00683	0.345	0.387
elt_000_15788	Cd ₃ Gd ₂ MgSb	7	-2.425	-2.75	-5.200e-05	0.00861	1.125	1.657
elt_000_15796	CaGa ₂ SnTb ₂	6	-3.633	-3.919	-4.000e-06	0.0034	0.919	1.049
elt_000_15805	Ga ₂ GeTb ₃	6	-4.21	-4.499	5.000e-06	0.00911	0.781	0.92
elt_000_15830	As ₃ Gd ₂ LaMo	7	-5.99	-6.484	-2.500e-05	0.00624	0.779	1.921
elt_000_15848	CaCdEuSbYb ₂	6	-2.159	-2.422	0.000e+00	0.00606	1.003	1.677
elt_000_15850	Ge ₂ Hf ₂ Mn ₂	6	-7.464	-8.146	-2.000e-05	0.00834	1.334	1.458
elt_000_15872	Au ₃ Nd ₂ Sr	6	-3.811	-4.177	1.000e-06	0.00504	0.713	1.078
elt_000_15906	CuDy ₂ NiTe ₂	6	-4.215	-4.761	-6.000e-06	0.00773	0.812	2.63
elt_000_15922	MoNd ₃ Si ₂	6	-5.854	-6.054	-2.000e-06	0.00629	0.307	1.663
elt_000_15993	AsGe ₂ Nd ₃	6	-4.834	-5.554	-2.900e-05	0.00531	1.361	2.032
elt_000_16005	AgMn ₂ MoSn ₂	6	-5.778	-6.195	0.000e+00	0.0033	0.95	1.28
elt_000_16023	PbSrTb ₂	4	-3.361	-3.741	0.000e+00	0.00338	1.319	2.402
elt_000_16054	Ga ₃ Nd ₃	6	-3.902	-4.294	0.000e+00	0.00565	1.235	1.391
elt_000_16106	Si ₃ Tb ₃	6	-5.111	-5.552	0.000e+00	0.00383	0.645	2.337
elt_000_16113	AlBaCo ₃ GaTb ₂	8	-4.77	-4.961	-2.100e-05	0.00626	0.596	0.906
elt_000_16122	As ₂ Gd ₂ P ₃ W	8	-5.81	-6.474	-1.000e-06	0.00581	1.149	2.236
elt_000_16123	As ₄ Gd ₂ HfV	8	-6.25	-6.454	-1.000e-06	0.00408	0.419	1.368
elt_000_16140	Ni ₂ Si ₂ TiW	6	-7.053	-7.438	-1.100e-05	0.00862	0.47	0.722
elt_000_16142	Ge ₃ LaNd ₂	6	-4.946	-5.284	1.000e-06	0.00696	0.692	0.964
elt_000_16147	Gd ₃ Sb ₃	6	-4.78	-5.316	0.000e+00	0.00217	1.037	2.119
elt_000_16156	CdSSe ₂ SrYb ₂	7	-3.395	-3.84	-8.000e-06	0.00587	1.395	2.053
elt_000_16202	Al ₅ Nd ₂	7	-3.751	-4.159	-1.000e-06	0.00404	1.27	0.938
elt_000_16220	Sn ₃ Ti ₂ Yb ₃	8	-3.769	-4.097	-4.000e-06	0.00858	0.913	1.502
elt_000_16254	As ₃ MoRu ₂	6	-7.054	-7.224	1.100e-05	0.00897	0.567	1.653
elt_000_16257	Gd ₃ Ge ₃ Rh	7	-5.334	-5.623	-4.000e-06	0.00766	0.856	2.091
elt_000_16266	CdPb ₃ Pt ₂ Yb ₂	8	-3.754	-3.706	0.000e+00	0.00519	0.354	0.972
elt_000_16272	BaGd ₂ RhSb	5	-4.643	-4.993	-1.000e-06	0.00472	0.639	0.742
elt_000_16275	AuGeSn ₂ YYb ₂	7	-3.773	-4.155	-2.000e-06	0.00476	1.162	1.434
elt_000_16296	Hg ₃ Tb ₃	6	-2.576	-2.847	-1.500e-05	0.00699	1.229	2.117
elt_000_16301	Al ₂ Ni ₃ W	6	-6.164	-6.368	-1.200e-05	0.00679	0.19	0.257

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_16319	As ₄ Gd ₂ TiV	8	-5.772	-6.067	-1.000e-06	0.00696	0.484	0.686
elt_000_16329	GeNd ₂ NiPd ₂ Sb	7	-4.922	-5.579	0.000e+00	0.00609	1.349	1.815
elt_000_16331	Pd ₂ Tb ₃ Zn	6	-4.547	-4.834	-1.000e-06	0.00477	0.764	1.023
elt_000_16334	Te ₂ Yb ₂	4	-2.829	-3.972	0.000e+00	0.00424	1.957	2.228
elt_000_16342	Cd ₂ Nd ₂ RbSb	6	-2.633	-2.906	-9.000e-06	0.00548	0.735	1.169
elt_000_16364	As ₂ CdDy ₂ Si	6	-4.317	-4.545	-1.000e-06	0.00191	0.37	0.538
elt_000_16366	Cu ₂ SbTb ₃	6	-4.392	-4.646	-3.700e-05	0.0069	0.824	0.776
elt_000_16384	CeGeSbTe ₃ Yb ₂	8	-3.817	-4.36	-3.600e-05	0.00399	0.711	1.923
elt_000_16412	Nd ₂ Se ₄	6	-4.912	-5.487	-6.000e-06	0.00804	1.271	2.25
elt_000_16448	As ₃ Nd ₃	6	-5.204	-5.922	-5.000e-06	0.00398	0.831	1.269
elt_000_16468	Ba ₄ MgNd ₂	7	-2.366	-2.561	-1.000e-06	0.00478	0.782	1.472
elt_000_16472	CdSb ₂ Tb ₃	6	-3.917	-4.466	-1.000e-06	0.00281	0.653	1.12
elt_000_16482	AuDy ₂ RuSbSn	6	-5.288	-5.523	-5.000e-06	0.00578	1.48	2.021
elt_000_16520	CdCo ₂ Dy ₂ SbZn	7	-4.156	-4.443	-1.700e-05	0.00549	0.724	0.825
elt_000_16533	Pt ₂ Ru ₂ SiTm	6	-6.691	-7.113	6.000e-06	0.00653	0.258	0.316
elt_000_16556	GaNbNiRu ₂ Si ₂	7	-6.914	-7.166	-1.000e-06	0.00778	0.806	0.973
elt_000_16560	Co ₂ PSeTeZr	6	-5.162	-6.048	-3.000e-06	0.0067	1.019	0.808
elt_000_16576	Dy ₂ Na ₂ Sb ₂ SrZn	8	-3.103	-3.324	-1.000e-06	0.00342	0.791	1.736
elt_000_16596	BaCoSb ₃ Yb ₂	7	-3.745	-4.146	1.000e-06	0.00357	1.162	2.929
elt_000_16607	As ₃ MoNi ₂	6	-5.129	-5.996	-9.000e-06	0.00685	0.988	0.991
elt_000_16615	Gd ₃ Sb ₃	6	-4.751	-5.317	0.000e+00	0.00331	0.852	1.15
elt_000_16662	Co ₂ Tb ₅	7	-5.232	-5.344	8.000e-06	0.00557	0.447	0.501
elt_000_16680	NaSb ₃ Tb ₂	6	-3.945	-4.489	-1.000e-06	0.0031	2.218	3.058
elt_000_16684	Cd ₂ GaSrYb ₂	6	-1.593	-1.758	-5.000e-06	0.00436	1.075	1.391
elt_000_16697	Nd ₂ NiPt ₂ Sn	6	-5.497	-5.915	2.000e-06	0.00697	1.051	1.309
elt_000_16706	AuGa ₂ Tb ₂ Y	6	-4.36	-4.666	-1.000e-06	0.00806	1.044	1.435
elt_000_16718	Ni ₂ Se ₂	4	-3.911	-4.426	-2.000e-06	0.00723	0.438	0.338
elt_000_16725	Dy ₂ SrZn ₃	6	-2.299	-2.493	-5.000e-06	0.00488	0.303	0.629
elt_000_16727	Fe ₃ PSbZn	6	-5.189	-5.606	-2.500e-05	0.00872	0.391	1.402
elt_000_16731	AlNd ₂ OsSiTe ₂	7	-5.11	-5.707	0.000e+00	0.00347	1.005	2.03
elt_000_16758	GeIr ₂ NaTb ₂	6	-5.401	-5.82	-5.000e-06	0.00952	1.426	2.118
elt_000_16765	Nd ₂ Sn ₃ Sr	6	-4.007	-4.328	-1.000e-06	0.00267	0.888	1.136
elt_000_16780	Fe ₂ Li ₂ MoSb	6	-5.174	-5.712	2.000e-06	0.00938	0.535	0.841
elt_000_16790	Dy ₂ NiRbTe ₃	7	-4.137	-4.561	-1.200e-05	0.00845	0.641	2.114
elt_000_16804	AgGaNdTb ₂	5	-3.935	-4.09	-9.000e-06	0.00752	0.425	0.543
elt_000_16812	Ga ₃ SrTb ₂	6	-3.321	-3.649	-2.000e-06	0.00533	1.182	2.77
elt_000_16859	GaPdSrTb ₂	5	-3.933	-4.114	-3.000e-06	0.00851	0.717	1.651
elt_000_16880	Co ₂ Ge ₂ La	5	-4.767	-5.889	-1.000e-06	0.00727	0.901	0.98
elt_000_16886	Ru ₂ SiSnYZn	6	-5.641	-6.013	0.000e+00	0.00182	0.751	0.878
elt_000_16897	Ga ₂ Gd ₂ SnYb	6	-3.597	-3.88	-3.000e-06	0.00645	0.893	1.015
elt_000_16904	AlDy ₃ PdZn	6	-4.102	-4.342	-1.000e-06	0.00385	0.64	0.851
elt_000_16908	Al ₂ SiSnYb ₃	7	-3.137	-3.235	0.000e+00	0.00526	0.299	0.325
elt_000_16910	Gd ₃ GeSi ₂	6	-4.97	-5.496	-1.000e-06	0.00581	1.001	3.01
elt_000_16912	CdDy ₂ Sb	4	-3.396	-4.097	1.000e-06	0.00439	1.36	1.699
elt_000_16931	Gd ₄ Ge ₃ Pt	8	-5.549	-5.695	0.000e+00	0.0077	0.426	0.601
elt_000_16936	Fe ₂ Nd ₃ NiSV	8	-6.209	-6.369	-3.000e-06	0.00757	0.384	0.471
elt_000_16939	Nd ₂ S ₃ SeSnZr	8	-5.505	-6.014	-2.000e-06	0.00246	0.819	1.54
elt_000_16946	SbSrYb ₂	4	-2.124	-2.679	8.000e-06	0.00257	1.301	2.509
elt_000_16953	GaNi ₃ Tb ₄	8	-4.675	-5.043	7.000e-06	0.00857	0.512	0.961
elt_000_16966	Dy ₂ GaTe ₄	7	-4.144	-4.401	0.000e+00	0.00855	0.469	0.587
elt_000_16975	Ni ₃ Sn ₂ Ti	6	-4.447	-5.409	-1.000e-06	0.00932	0.81	1.682
elt_000_16984	Au ₃ Nd ₄	7	-4.411	-4.697	0.000e+00	0.0052	0.505	1.453

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_16988	Cu ₂ GaTb ₃	6	-4.038	-4.248	-3.000e-06	0.0053	0.459	0.51
elt_000_17027	As ₃ Co ₂ Mo	6	-5.507	-6.451	-4.000e-06	0.00663	0.441	0.639
elt_000_17053	AlDy ₃ Ge ₂	6	-4.775	-4.992	0.000e+00	0.0073	1.078	1.172
elt_000_17064	AgCdDy ₂ GaSnW ₂	8	-4.865	-5.621	-1.000e-06	0.00747	0.984	1.569
elt_000_17068	BaGd ₂ Sb ₃	6	-4.25	-4.891	-4.000e-06	0.0035	1.005	1.279
elt_000_17084	AsGeRuSnTb ₂ Te	7	-5.022	-5.298	-3.000e-06	0.00978	0.307	0.577
elt_000_17088	AsMn ₂ P ₂ W	6	-7.507	-7.769	-1.700e-05	0.00553	0.435	0.567
elt_000_17095	AsCeNd ₂ PtRhSn	7	-5.686	-6.06	-4.000e-06	0.00435	0.68	0.938
elt_000_17097	CoGe ₂ LaTb ₂	6	-5.184	-5.555	0.000e+00	0.00696	0.901	1.153
elt_000_17113	Gd ₃ Ge ₃	6	-4.822	-5.192	-3.000e-06	0.00433	0.656	0.862
elt_000_17114	AuGaRhTb ₃ Te	7	-4.838	-4.999	1.000e-06	0.00518	0.448	0.615
elt_000_17152	BaGeNd ₂ SnZn	6	-3.582	-3.814	-1.000e-06	0.00436	0.41	1.282
elt_000_17159	CaGa ₃ Yb ₂	6	-2.423	-2.67	-5.000e-06	0.008	0.969	2.045
elt_000_17174	Pt ₆ Ru ₂	8	-6.444	-6.77	-1.000e-06	0.00279	0.458	0.53
elt_000_17176	Co ₂ MnTe	4	-5.623	-6.107	-6.000e-06	0.00772	1.134	2.273
elt_000_17181	Al ₃ Nb ₃ Nd ₂	8	-6.144	-6.423	-1.000e-06	0.00463	0.613	1.464
elt_000_17205	AuGa ₂ Gd ₂ OsSn	7	-5.011	-5.204	-1.400e-05	0.00396	0.779	0.912
elt_000_17218	Ge ₃ PtScTb ₂	7	-5.296	-5.764	-3.000e-06	0.00967	1.048	1.4
elt_000_17225	FeGeNi ₂ Si ₂	6	-5.504	-5.942	0.000e+00	0.00792	0.784	1.041
elt_000_17228	Cd ₂ Gd ₃ Ni ₂	7	-3.847	-3.991	-5.600e-05	0.00574	0.631	0.829
elt_000_17231	RbSb ₃ Yb ₂	6	-2.913	-3.302	0.000e+00	0.00616	1.014	1.825
elt_000_17247	BeMnNi ₂ ScSi	6	-5.871	-6.003	-2.400e-05	0.00748	0.292	0.504
elt_000_17259	SnTeYb ₂	4	-2.651	-3.407	-1.600e-05	0.00611	1.838	2.532
elt_000_17270	Pr ₂ RhSn ₂ Yb ₂	7	-4.278	-4.559	-2.000e-06	0.00699	1.314	1.611
elt_000_17275	CdMgNiSnTb ₂	6	-3.559	-3.777	0.000e+00	0.0062	0.28	0.429
elt_000_17279	I ₂ Mn ₂ Se ₂	6	-4.235	-4.704	-3.000e-06	0.00679	1.002	0.61
elt_000_17305	Nd ₃ Pt ₂ Sn	6	-5.668	-5.964	0.000e+00	0.00205	0.874	1.154
elt_000_17307	As ₂ FeTb ₃ TeZn	8	-4.35	-5.089	1.000e-06	0.0086	0.722	0.753
elt_000_17310	CoDy ₃ Ga ₂	6	-4.421	-4.822	0.000e+00	0.00862	1.624	2.586
elt_000_17315	Ge ₄ Mn ₂	6	-5.169	-5.923	-1.000e-06	0.00379	0.608	0.842
elt_000_17322	Pt ₂ SbYb ₃	6	-4.102	-4.469	-4.000e-06	0.00683	0.875	0.999
elt_000_17359	CdCsNd ₂ SnTe	6	-3.151	-3.518	-9.000e-06	0.00563	1.744	3.578
elt_000_17360	CaPtSi ₂ Tb ₂	6	-4.95	-5.353	0.000e+00	0.00494	0.969	2.047
elt_000_17366	Cu ₃ Dy ₂ V	6	-4.418	-4.826	-7.000e-06	0.00625	0.444	0.862
elt_000_17371	AlNiTb ₃ Zn ₂	7	-3.664	-3.918	7.000e-06	0.00541	0.986	1.569
elt_000_17404	Nd ₃ S ₄ Zr	8	-6.407	-6.726	-2.000e-06	0.00511	0.753	0.683
elt_000_17414	Ag ₂ Dy ₂ Mn ₂ Nd	7	-4.939	-5.179	2.000e-06	0.0077	0.875	1.023
elt_000_17428	Ni ₂ PtTb ₃	6	-5.326	-5.748	-4.500e-05	0.00725	0.697	1.078
elt_000_17442	CaDy ₂ Ga ₂ Pd	6	-3.967	-4.232	0.000e+00	0.00587	0.406	0.523
elt_000_17457	AuDy ₃ Zn	5	-3.798	-3.89	0.000e+00	0.00345	0.321	0.232
elt_000_17532	Ga ₂ Nd ₃ NiZn	7	-3.994	-4.152	-4.300e-05	0.00594	0.932	1.307
elt_000_17553	GaGd ₃ NiZn	6	-4.008	-4.217	-1.000e-06	0.00536	1.26	0.909
elt_000_17564	AlDy ₃ Pt	5	-4.891	-5.229	1.000e-06	0.00345	0.44	0.551
elt_000_17571	AuGd ₂ Hg ₂ ITe	7	-2.931	-3.112	-1.000e-06	0.00467	1.207	1.269
elt_000_17591	Al ₂ Dy ₂ SnZn	6	-3.647	-3.943	-9.000e-06	0.00914	0.874	1.004
elt_000_17648	Au ₂ GaYb ₃	6	-2.725	-3.015	-1.000e-06	0.00523	0.67	1.104
elt_000_17690	Ga ₂ GeNd ₃	6	-4.193	-4.572	1.000e-06	0.00704	1.006	1.078
elt_000_17714	GaGeRuTb ₃	6	-5.193	-5.585	-1.400e-05	0.00869	0.795	1.077
elt_000_17718	AsMgMn ₂ Ni ₂ P ₂	8	-5.173	-5.852	-2.000e-06	0.00393	1.071	1.123
elt_000_17722	Sb ₃ Yb ₃	6	-3.226	-3.621	-3.000e-06	0.00579	0.648	2.214
elt_000_17729	Mn ₂ PtReSiW	6	-8.874	-9.168	-8.000e-06	0.00737	0.202	0.224
elt_000_17754	As ₃ MoNi ₂	6	-5.212	-5.998	1.000e-06	0.00897	0.671	1.934

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_17762	Cr ₂ Nd ₂ Te ₂	6	-5.22	-6.005	-8.000e-06	0.00508	1.458	1.859
elt_000_17780	BrIPtYb ₂	5	-2.708	-3.767	-2.500e-05	0.00443	2.023	3.839
elt_000_17783	Mn ₂ PdSn	4	-5.936	-6.548	-3.440e-04	0.00818	0.708	0.81
elt_000_17803	Au ₃ SbYb ₂	6	-3.126	-3.569	-1.000e-06	0.00436	1.401	2.098
elt_000_17808	Al ₃ GeYb ₄	8	-2.828	-3.034	-2.000e-06	0.00327	0.584	1.579
elt_000_17818	Co ₃ Ga ₂ Ge	6	-4.897	-5.215	-4.000e-06	0.00643	0.288	0.311
elt_000_17822	Cd ₄ Nd ₂ SbSm	8	-2.703	-2.95	-1.300e-05	0.00478	0.785	0.973
elt_000_17852	Co ₂ Fe ₂ Si ₂	6	-6.946	-7.113	-2.800e-05	0.00931	0.478	0.558
elt_000_17873	Dy ₃ OsRhSi ₂	7	-6.421	-6.764	1.000e-06	0.00513	0.97	1.738
elt_000_17921	HgNd ₂ Y	4	-3.919	-4.221	-6.000e-06	0.006	1.129	1.642
elt_000_17933	InSb ₂ Yb ₃	6	-3.048	-3.21	0.000e+00	0.00546	0.714	0.913
elt_000_17936	HgSrTb ₂	4	-2.606	-2.93	-3.000e-06	0.00276	1.03	1.306
elt_000_17958	Ga ₂ NaYb ₃	6	-1.965	-2.09	-1.000e-06	0.0043	0.491	0.823
elt_000_17964	CoFe ₂ Ga ₂ Sn	6	-4.901	-5.329	-6.000e-06	0.00563	0.372	0.716
elt_000_17978	Al ₃ CaDy ₃	7	-3.748	-4.007	-4.000e-06	0.00366	0.44	0.532
elt_000_17991	AlCeGa ₂ Gd ₂	6	-4.236	-4.501	-6.900e-05	0.00805	0.905	1.05
elt_000_18013	GaGd ₃ Os ₃	7	-6.92	-7.258	-5.000e-06	0.00823	0.737	0.85
elt_000_18020	AlCaCd ₂ Gd ₂ Ge ₂	8	-3.292	-3.468	0.000e+00	0.006	0.519	1.497
elt_000_18028	Co ₃ Dy ₃	6	-5.434	-5.844	-1.000e-06	0.00882	0.716	1.821
elt_000_18038	CsDy ₂ NiSb ₂ Sn	7	-4.233	-4.43	-8.000e-06	0.00675	0.472	0.686
elt_000_18039	Fe ₂ Mg ₃ Y	6	-3.952	-4.313	-1.000e-06	0.00938	0.756	0.642
elt_000_18068	CrGe ₂ Nd ₃ Ni	7	-5.448	-5.606	-5.000e-06	0.00757	0.451	0.616
elt_000_18121	Dy ₃ GePd ₂	6	-5.337	-5.502	-3.000e-06	0.00618	0.711	0.79
elt_000_18125	FeNd ₃ Si ₃	7	-5.689	-5.913	-8.000e-06	0.00762	0.841	0.939
elt_000_18127	Fe ₃ GaY	5	-5.917	-6.626	-1.000e-06	0.00611	0.392	0.581
elt_000_18129	AsCo ₂ HfMn ₂	6	-7.541	-7.707	-3.400e-05	0.0083	0.306	0.386
elt_000_18142	As ₃ CeKNYb ₂	8	-4.427	-4.821	-1.700e-05	0.00962	1.023	1.06
elt_000_18147	Sn ₃ SrYb ₂	6	-2.895	-3.203	-1.000e-06	0.00638	1.13	1.288
elt_000_18176	As ₃ SrTb ₂ Zn	7	-4.157	-4.639	0.000e+00	0.00399	1.018	2.726
elt_000_18190	PtRu ₂ Si ₃ Y	7	-7.036	-7.466	-2.000e-06	0.00542	0.597	0.743
elt_000_18194	As ₂ CdITb ₂ Te	7	-3.881	-4.226	-1.600e-05	0.00684	0.299	0.729
elt_000_18196	CdGd ₃ Mg	5	-3.175	-3.332	0.000e+00	0.0011	0.713	2.184
elt_000_18200	As ₃ Dy ₂ Te	6	-4.634	-5.226	-1.000e-06	0.00452	1.077	2.012
elt_000_18212	MgNd ₂ Sn ₂ Sr ₃	8	-2.97	-3.236	1.000e-06	0.00301	0.812	1.19
elt_000_18213	Al ₃ FeYb ₃	7	-3.271	-3.386	-7.000e-06	0.00786	0.649	0.772
elt_000_18217	AuCdSb ₂ Yb ₃	7	-2.87	-3.003	0.000e+00	0.00546	0.876	2.073
elt_000_18218	AsCaGeNd ₂ Te	6	-4.185	-4.97	-1.000e-06	0.00902	0.87	1.337
elt_000_18225	Dy ₂ Ga ₃ Pr	6	-3.866	-4.247	-7.000e-06	0.00571	0.762	1.802
elt_000_18274	AuBiRu ₂ SnTb ₂	7	-5.647	-5.858	4.000e-06	0.00561	0.713	1.264
elt_000_18275	AlCd ₃ Dy ₂ Pd	7	-2.994	-3.292	-8.000e-06	0.00814	1.104	2.447
elt_000_18314	Co ₂ Ga ₂ Tb ₃	7	-4.748	-5.095	0.000e+00	0.00609	0.882	1.36
elt_000_18318	Ga ₂ Nd ₃	5	-4.176	-4.323	-1.000e-06	0.00657	0.564	1.785
elt_000_18337	Dy ₃ GaPt ₂	6	-5.425	-5.746	-1.000e-06	0.00143	0.841	1.162
elt_000_18338	Nd ₂ Te ₄	6	-4.087	-4.738	-2.000e-06	0.0057	2.139	2.198
elt_000_18339	GeNd ₃ SnTe ₂	7	-4.702	-4.908	0.000e+00	0.00789	0.471	2.773
elt_000_18374	AuCaHg ₂ Nd ₂	6	-2.742	-3.091	0.000e+00	0.0041	1.433	2.493
elt_000_18375	Au ₂ Co ₂ Mg ₂	6	-3.514	-3.965	0.000e+00	0.0074	0.755	0.873
elt_000_18379	Dy ₂ K ₂ O ₄	8	-6.21	-6.648	-9.000e-06	0.00531	0.87	1.454
elt_000_18385	Dy ₃ InSi ₃	7	-4.811	-5.026	0.000e+00	0.00461	0.847	0.845
elt_000_18404	Gd ₅ GePtRu	8	-5.598	-5.85	1.000e-06	0.00402	0.589	0.829
elt_000_18464	Gd ₂ Sb ₂ SnSr	6	-4.078	-4.592	-5.000e-06	0.00604	0.88	1.016
elt_000_18473	BaGd ₂ RhSn	5	-4.403	-4.844	0.000e+00	0.00478	0.872	0.694

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
elt_000_18508	AlDy ₃ Ni	5	-4.448	-4.779	-2.000e-05	0.00366	0.411	0.547
elt_000_18520	Ge ₃ Ru ₂ Sc	6	-6.051	-6.62	0.000e+00	0.00973	0.478	0.59
elt_000_18535	AlCoSiTb ₄	7	-4.928	-5.218	-9.000e-06	0.00568	0.747	0.785
elt_000_18539	Au ₂ Dy ₂ SnSr	6	-4.049	-4.175	-2.000e-06	0.00388	0.727	1.911
elt_000_18554	AuGd ₃ P ₂ Sn	7	-5.13	-5.451	0.000e+00	0.00355	0.209	0.509
elt_000_18558	BaNd ₂ Si ₃	6	-4.565	-5.002	-2.000e-06	0.00313	0.581	0.945
elt_000_18566	Ge ₃ PrRu ₂	6	-6.048	-6.41	-1.000e-06	0.00403	0.824	0.985
elt_000_18590	CaDy ₂ Ga ₃	6	-3.436	-3.739	-3.000e-06	0.00703	1.001	1.171
elt_000_18596	Co ₃ GePV	6	-6.528	-6.874	-5.000e-06	0.00905	0.879	1.471
elt_000_18616	Tb ₂ Te ₃	5	-4.265	-4.93	0.000e+00	0.00781	1.281	2.154
elt_000_18628	Au ₃ ITb ₂	6	-3.643	-4.017	0.000e+00	0.00246	1.257	2.738
elt_000_18646	Pt ₅ Tb ₃	8	-6.218	-6.383	1.000e-06	0.00869	0.496	1.331
elt_000_18669	Dy ₂ GeI ₂ LaRhRu	8	-4.97	-5.33	-6.000e-06	0.00863	0.68	0.918
elt_000_18673	LiRhRu ₂	4	-6.437	-6.823	-1.000e-06	0.00485	0.472	0.365
elt_000_18730	CoGaGeSTb ₂ Te	7	-4.532	-4.906	0.000e+00	0.00512	0.585	0.701
elt_000_18760	Al ₂ AsGd ₃ RhW	8	-5.831	-6.132	-6.000e-06	0.00322	0.607	0.847
elt_000_18765	Al ₂ AsEuGd ₂ GeRh	8	-4.761	-5.097	0.000e+00	0.00589	1.187	1.436
elt_000_18772	Ge ₂ Tb ₂ TeU	6	-5.227	-5.952	3.000e-06	0.00585	1.085	2.305
elt_000_18803	Ga ₄ Mn ₂	6	-4.512	-4.938	3.000e-06	0.00804	0.458	0.656
elt_000_18861	As ₃ Dy ₂ Eu	6	-4.6	-5.288	0.000e+00	0.00345	0.682	1.092
elt_000_18869	Dy ₄ PdSn ₂	7	-4.939	-5.022	-1.000e-06	0.00386	0.478	0.62
elt_000_18912	Gd ₂ Sb ₃ Sr	6	-4.307	-4.884	0.000e+00	0.00445	0.921	1.413
elt_000_18928	Dy ₄ Pd ₂ Sn ₂	8	-5.182	-5.309	-5.000e-06	0.00344	0.504	0.525
elt_000_18949	Ge ₂ Mn ₂ SbTm	6	-5.702	-5.962	-9.000e-06	0.00831	0.733	0.821
elt_000_18985	Nd ₂ Rh ₃ Sr	6	-5.459	-5.828	3.000e-06	0.00607	0.845	1.067
elt_000_18995	Cd ₃ Dy ₄ Pb	8	-3.208	-3.293	0.000e+00	0.0072	0.355	0.358
elt_000_19009	AlMgNi ₂ SmTb ₃	8	-4.518	-4.613	-4.200e-05	0.0052	0.42	2.568
elt_000_19034	GeNd ₃ Pt ₂	6	-5.743	-5.962	0.000e+00	0.00723	0.829	2.87
elt_000_19037	Dy ₂ Ga ₂ Nd	5	-4.032	-4.254	-1.000e-06	0.0067	0.493	0.453
elt_000_19052	Pd ₃ Yb ₄	7	-3.679	-3.821	-2.000e-06	0.00238	0.451	0.497
elt_000_19074	BNiPRh ₂ Ru ₂	7	-6.925	-7.364	-2.000e-06	0.00708	0.584	1.719
elt_000_19078	Gd ₂ Ni ₃ Sn ₂	7	-4.865	-5.239	0.000e+00	0.00911	0.874	0.905
elt_000_19110	Co ₃ Mn ₂ NdSi ₂	8	-6.355	-7.049	-6.000e-06	0.0056	1.553	2.849
elt_000_19122	Au ₃ Dy ₃	6	-4.238	-4.761	0.000e+00	0.0044	1.387	3.189
elt_000_19127	Co ₃ Ge ₂ Te	6	-4.899	-5.435	-2.000e-06	0.00825	0.853	1.554
elt_000_19153	Gd ₃ Ge ₃	6	-4.728	-5.19	-4.000e-06	0.00997	0.525	0.749
elt_000_19154	MoNd ₂ P ₃ Sb ₂	8	-5.775	-6.094	-4.000e-06	0.00852	0.643	1.13
elt_000_19170	BaGd ₂ NiSn ₃	7	-4.293	-4.544	-3.000e-06	0.00523	0.823	0.985
elt_000_19180	AgCuDy ₂ Ga ₂	6	-3.64	-3.953	-3.700e-05	0.00797	0.862	0.888
elt_000_19202	BrPtRbTb ₂	5	-3.46	-4.353	1.000e-06	0.00624	2.122	3.194
elt_000_19205	PRu ₂ Sn ₃	6	-4.038	-5.936	-3.000e-06	0.0073	0.776	0.846
elt_000_19219	Ni ₂ SnYb ₃ Zn	7	-3.078	-3.308	-6.000e-06	0.00638	0.907	0.489
elt_000_19220	Co ₂ Se ₂ Ti ₂	6	-5.74	-6.536	0.000e+00	0.00939	0.824	1.185
elt_000_19226	BiCuDy ₂ Ga ₃	7	-3.875	-4.137	-2.000e-06	0.00561	0.945	1.053
elt_000_19230	HfNd ₂ SbSe ₃	7	-5.812	-6.061	-2.000e-06	0.00367	0.488	0.701
elt_000_19244	Dy ₂ MgTe ₃	6	-3.941	-4.319	-1.000e-06	0.0041	1.005	1.426
elt_000_19246	CAsBGd ₃ Os ₂	8	-7.023	-7.581	0.000e+00	0.00669	1.282	1.995
elt_000_19258	AsFe ₃ Ga ₂	6	-5.535	-5.745	-1.200e-05	0.00759	0.328	0.262
elt_000_19269	BaSb ₂ Yb ₃	6	-2.908	-3.111	0.000e+00	0.00319	0.845	0.96
elt_000_19289	CdSb ₃ Tb ₂ Tl	7	-3.638	-3.9	0.000e+00	0.00522	0.644	1.879
elt_000_19307	Mn ₂ Re ₄	6	-10.799	-11.127	-5.000e-06	0.00893	0.38	0.51
elt_000_19326	Ni ₄ Zn	5	-4.221	-4.669	-4.000e-06	0.00264	0.524	0.744

Table S8. The profile of generated materials with Elongated triangular lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E_{start}	E_{final}	E_{conv}	F_{max}	d_{latt}	d_{xy}
elt_000_19368	Ga ₂ Gd ₂ NiSbTb	7	-4.5	-4.686	-7.000e-06	0.00557	0.932	0.964
elt_000_19369	AsBaPtTb ₂	5	-4.681	-5.187	-4.000e-06	0.00519	1.119	1.139
elt_000_19371	CeGe ₂ Nd ₂ Pd ₃	8	-5.359	-5.753	0.000e+00	0.00421	0.922	1.934
elt_000_19372	Al ₄ NdRu ₂	7	-5.379	-5.712	6.000e-06	0.00803	0.531	0.806

Table S9. The profile of generated materials with Snub square lattice structures after DFT relaxation

Index	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sns_000_00001	Au ₃ Pd ₂ Yb ₈	13	-3.07	-3.198	2.000e-06	0.00317	0.408	0.964
sns_000_00013	Gd ₆ Ge ₇ Pd ₃	16	-5.131	-5.382	0.000e+00	0.00865	0.646	1.382
sns_000_00021	Al ₂ Dy ₈	10	-4.218	-4.429	2.000e-06	0.00189	1.052	1.375
sns_000_00033	Ga ₅ Nb ₃ Ru ₆	14	-7.194	-7.497	0.000e+00	0.00377	0.818	0.958
sns_000_00049	Al ₈ Nd ₆ Sn	15	-4.112	-4.453	0.000e+00	0.00455	0.499	1.307
sns_000_00052	Tb ₄ Tl ₂	6	-3.594	-3.968	-1.000e-06	0.00395	0.843	0.983
sns_000_00084	As ₂ CoFeMn ₅ Sc ₃ Si ₃	15	-6.906	-7.248	0.000e+00	0.00379	0.689	1.282
sns_000_00088	Ga ₇ GeNd ₄ Ru ₄	16	-5.143	-5.43	0.000e+00	0.00479	0.982	2.525
sns_000_00090	Ga ₄ Nd ₆ Ni ₃ Pr ₂	15	-4.656	-4.733	2.000e-06	0.00709	0.325	0.351
sns_000_00102	Dy ₇ Pd ₃ Yb ₃	13	-4.17	-4.342	0.000e+00	0.00501	0.818	0.882
sns_000_00110	CaGa ₇ NaNd ₆	15	-3.74	-3.877	-2.000e-06	0.00375	0.297	1.302
sns_000_00112	Gd ₇ Sn ₇ Sr	15	-4.394	-4.635	-3.000e-06	0.00248	0.394	1.191
sns_000_00116	Al ₈ Gd ₇ Tb	16	-4.334	-4.563	-5.000e-06	0.00516	0.363	0.682
sns_000_00122	Ge ₂ Ni ₄ Ru ₄ SiSrTb	13	-6.001	-6.258	-4.200e-05	0.00881	0.903	2.841
sns_000_00145	Dy ₅ Ga ₉ PdSn	16	-3.828	-4.143	-3.000e-06	0.0047	1.523	2.399
sns_000_00198	Bi ₄ Pb ₂ Yb ₁₀	16	-2.853	-2.945	-3.000e-06	0.00293	0.436	0.573
sns_000_00204	Nd ₆ Sb ₉	15	-4.791	-5.138	-9.000e-06	0.00711	1.634	2.757
sns_000_00218	GaRu ₆ Sn ₇	14	-5.517	-6.112	1.000e-06	0.00457	0.499	0.637
sns_000_00231	Ga ₄ GeMn ₇ Rh ₄	16	-6.615	-6.796	0.000e+00	0.00743	0.566	2.27
sns_000_00241	Ni ₅ Sn ₂ Tb ₆	13	-5.07	-5.205	-1.800e-05	0.00988	0.663	0.874
sns_000_00275	Gd ₈ Ir ₄ OsSb ₂	15	-6.597	-6.765	0.000e+00	0.0099	0.338	0.835
sns_000_00285	Al ₈ LaYb ₆	15	-2.921	-3.021	-4.000e-06	0.00452	0.555	0.552
sns_000_00303	AsNb ₂ P ₅ Ru ₆	14	-7.669	-7.99	0.000e+00	0.00534	0.598	0.53
sns_000_00366	Ru ₆ Zr ₇	13	-8.667	-9.085	0.000e+00	0.00763	0.965	2.042
sns_000_00415	AuFe ₅ PSb ₂	9	-5.88	-6.269	0.000e+00	0.00812	1.123	2.54
sns_000_00426	Fe ₇ Ga ₅ NbTiVZn	16	-6.081	-6.473	-1.000e-05	0.00468	1.276	1.259
sns_000_00456	Au ₃ Ga ₇ Nd ₄ U ₂	16	-4.447	-4.796	0.000e+00	0.00823	1.256	2.11
sns_000_00475	ClCs ₂ SbSeSnTe ₃ Yb ₄	13	-3.02	-3.577	0.000e+00	0.00517	0.976	3.112
sns_000_00476	CdGeSb ₄ Yb ₉	15	-2.789	-3.106	-5.000e-06	0.00571	1.631	2.274
sns_000_00478	Dy ₈ Ga ₆ Mg ₂	16	-3.713	-3.886	-4.000e-06	0.00582	0.927	0.933
sns_000_00483	Cd ₉ Nd ₇	16	-2.646	-2.781	2.000e-06	0.00596	1.063	1.085
sns_000_00519	FeGaNbNi ₁₂	15	-5.656	-5.791	-2.000e-06	0.00493	0.224	0.975
sns_000_00527	Ge ₆ Ru ₄ Tb ₄ U	15	-6.483	-6.609	-1.000e-06	0.0071	0.209	0.327
sns_000_00535	Cd ₂ Rh ₂ Yb ₈	12	-2.557	-2.628	-1.900e-05	0.00363	0.561	0.478
sns_000_00558	Ga ₂ Gd ₆ Ni ₅	13	-4.801	-4.993	1.000e-06	0.00719	0.52	0.526
sns_000_00583	Fe ₂ NiRu ₉ SiZr ₂	15	-8.221	-8.488	-1.000e-05	0.00835	0.221	0.5
sns_000_00609	Cd ₂ Dy ₆	8	-3.548	-3.723	-1.000e-06	0.00299	0.373	0.671
sns_000_00613	Co ₅ Ga ₃ La	9	-5.345	-5.549	3.000e-06	0.0087	0.339	1.057
sns_000_00645	Fe ₂ LiNi ₁₀ Si ₃	16	-5.488	-5.729	-1.000e-06	0.00444	0.409	0.41
sns_000_00671	Ge ₉ Nd ₆	15	-4.831	-5.085	-5.000e-06	0.00674	0.774	0.753
sns_000_00684	Co ₄ Tb ₁₀	14	-5.246	-5.376	-2.230e-04	0.00665	0.575	1.262
sns_000_00691	Co ₅ NaP ₂ Te	9	-5.144	-5.54	-2.600e-05	0.00922	0.698	0.656
sns_000_00707	Al ₃ Fe ₂ P ₄ PrRu ₄	14	-6.497	-6.922	6.000e-06	0.00629	0.461	1.531
sns_000_00708	Co ₅ Gd ₇ Ge	13	-5.481	-5.624	-6.000e-06	0.00487	0.482	0.984
sns_000_00709	Dy ₇ Pd ₅ Sb	13	-5.383	-5.453	-3.000e-06	0.00754	0.298	0.823
sns_000_00765	Dy ₁₀ Ga ₆	16	-4.363	-4.415	-1.000e-06	0.00322	0.304	0.216
sns_000_00775	Ga ₇ GeYb ₈	16	-2.487	-2.709	-1.500e-05	0.00676	0.58	1.697
sns_000_00789	CdDy ₇ Ga ₃ Pd ₃	14	-4.369	-4.623	1.000e-06	0.00541	0.574	0.766
sns_000_00804	Co ₈ Sn ₅	13	-5.351	-5.608	3.000e-06	0.00971	0.555	1.285
sns_000_00806	Gd ₈ Rh ₅	13	-6.115	-6.194	8.000e-06	0.00726	0.348	0.413
sns_000_00821	Ni ₂ PRu ₉ Si ₂	14	-7.363	-7.894	0.000e+00	0.00649	0.325	0.434
sns_000_00829	Gd ₇ Ge ₈ La	16	-5.126	-5.438	1.000e-06	0.00349	0.759	0.821

Table S9. The profile of generated materials with Snub square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sns_000_00830	CoGd ₆ Se ₈	15	-5.453	-5.8	-3.400e-05	0.00918	1.727	4.045
sns_000_00838	Al ₃ Ru ₁₁ Y	15	-7.713	-7.991	-1.000e-05	0.00544	0.582	0.724
sns_000_00853	Nd ₆ Sn ₇	13	-4.522	-4.872	-1.000e-06	0.00438	1.263	2.195
sns_000_00865	Ga ₈ Tb ₈	16	-4.111	-4.318	0.000e+00	0.00674	0.558	1.154
sns_000_00879	Ge ₃ Nd ₄ Pd ₂ Sn ₃ Tl ₄	16	-4.176	-4.341	-6.000e-06	0.00387	1.022	1.733
sns_000_00898	Al ₄ CuFe ₄ Ti ₇	16	-6.682	-6.929	0.000e+00	0.0036	0.811	1.322
sns_000_00918	Co ₁₃ V ₃	16	-7.262	-7.395	0.000e+00	0.00573	0.297	0.443
sns_000_00933	Os ₅ RhSi ₂ Tb ₇	15	-7.157	-7.386	1.000e-05	0.00467	0.68	1.133
sns_000_00940	Ga ₈ Gd ₇	15	-4.001	-4.161	1.000e-06	0.00524	0.517	0.399
sns_000_00964	Al ₅ Cu ₂ Ga ₂ Gd ₅	14	-3.953	-4.288	-2.000e-06	0.00553	1.15	2.983
sns_000_00984	Au ₇ Ga ₂ Gd ₄ Tl ₂	15	-3.397	-3.914	-2.000e-06	0.00589	0.801	1.93
sns_000_00989	Dy ₆ GePd ₅ Sb	13	-5.632	-5.496	0.000e+00	0.00667	0.858	1.107
sns_000_00996	Li ₂ Nd ₈ Si ₆	16	-4.961	-5.142	0.000e+00	0.00721	0.424	0.996
sns_000_01012	Mg ₂ Ni ₄ SbTb ₇	14	-4.57	-4.661	2.000e-06	0.0087	0.272	0.497
sns_000_01021	Dy ₁₀ Ga ₅	15	-4.185	-4.369	1.000e-06	0.00527	0.62	0.445
sns_000_01031	Au ₂ Cd ₂ Ir ₂ Nd ₉ Rh	16	-5.086	-5.141	-1.000e-06	0.00503	0.093	0.215
sns_000_01032	CeGe ₁₀ Yb ₅	16	-3.834	-4.122	0.000e+00	0.0049	0.69	0.814
sns_000_01046	Ga ₇ Gd ₇ Tb	15	-4.175	-4.341	1.000e-06	0.00288	0.248	1.243
sns_000_01048	Gd ₄ Pd ₅ Sn ₄	13	-4.961	-5.26	-5.000e-06	0.00411	0.988	1.783
sns_000_01051	Ga ₁₀ Nd ₅ Pd	16	-3.966	-4.072	-1.000e-06	0.00487	0.251	0.471
sns_000_01056	Gd ₆ HoIn ₄ LaSb ₃	15	-4.371	-4.507	-1.000e-06	0.00731	0.589	1.105
sns_000_01073	Al ₃ MoRu ₄ Si ₂ W	11	-7.504	-7.712	3.000e-06	0.00614	0.48	1.59
sns_000_01113	Na ₂ Ni ₄	6	-3.544	-3.846	-1.840e-04	0.00912	0.79	0.808
sns_000_01125	NaS ₇ Tb ₆ Tl	15	-5.335	-5.5	-1.400e-05	0.00429	0.495	0.763
sns_000_01165	Ge ₅ Li ₂ Pd ₂ Tb ₇	16	-4.805	-4.959	0.000e+00	0.00647	0.247	0.838
sns_000_01172	Ni ₄ Sn ₂	6	-4.788	-4.943	0.000e+00	0.00612	0.6	0.642
sns_000_01185	Ga ₁₁ Yb ₅	16	-2.687	-2.851	-1.000e-06	0.00921	0.497	0.574
sns_000_01187	AlCoNi ₁₄	16	-5.385	-5.506	-3.800e-05	0.00943	0.342	0.382
sns_000_01215	Al ₆ Dy ₄ Ru ₄ Sb ₂	16	-5.541	-5.797	-4.400e-05	0.00507	0.717	1.619
sns_000_01217	Gd ₁₀ Si ₅	15	-5.237	-5.301	0.000e+00	0.00354	0.244	0.372
sns_000_01278	As ₂ Co ₆	8	-6.399	-6.465	0.000e+00	0.00451	0.08	0.108
sns_000_01307	Al ₂ Ba ₂ Dy ₄ Ga ₃ Sn ₃	14	-3.677	-3.973	0.000e+00	0.00551	1.159	2.209
sns_000_01333	IrSi ₇ Tb ₈	16	-5.537	-5.763	-4.000e-06	0.00327	1.043	2.598
sns_000_01336	Nd ₇ Ni ₂ PtSn ₅	15	-4.76	-5.135	1.000e-06	0.00295	0.854	2.957
sns_000_01338	Eu ₂ CaFe ₅ Ga ₅ MgZn	15	-4.108	-4.429	0.000e+00	0.00741	1.45	1.995
sns_000_01396	CdHgMgNd ₄ Sb	8	-3.021	-3.642	0.000e+00	0.00728	1.855	3.128
sns_000_01408	Pd ₄ Yb ₈	12	-3.211	-3.316	-4.000e-06	0.00267	0.487	0.315
sns_000_01427	Ga ₇ Gd ₈	15	-4.052	-4.243	-5.000e-06	0.00677	0.571	1.027
sns_000_01433	Ge ₃ Mn ₁₁ P ₂	16	-7.527	-7.708	0.000e+00	0.00515	0.557	2.97
sns_000_01447	Co ₅ Ga ₄ Nd ₆	15	-4.976	-5.176	1.900e-05	0.0061	0.542	0.748
sns_000_01449	CeDy ₆ Ga ₅ Y	13	-4.405	-4.518	0.000e+00	0.0032	0.065	1.872
sns_000_01483	Pt ₄ Sb ₂ Yb ₈	14	-3.89	-3.977	0.000e+00	0.00502	0.488	0.685
sns_000_01495	As ₃ Nd ₆ Pt ₃	12	-5.553	-5.888	-7.000e-06	0.0055	1.142	2.216
sns_000_01503	GeSi ₆ Tb ₈	15	-5.243	-5.466	-1.000e-06	0.00317	0.338	0.489
sns_000_01509	Ga ₆ LiPt ₃ Tb ₆	16	-4.467	-4.741	0.000e+00	0.00556	1.063	1.455
sns_000_01524	Ru ₄ Tl ₄	8	-4.733	-5.382	0.000e+00	0.00704	1.207	1.422
sns_000_01542	Al ₉ Dy ₄ La ₃	16	-4.214	-4.557	-1.000e-06	0.00193	0.401	0.499
sns_000_01543	Ga ₃ La ₇ Ru ₆	16	-6.171	-6.353	0.000e+00	0.00838	1.188	3.171
sns_000_01548	Ge ₈ Ni ₂ Tb ₆	16	-5.04	-5.204	0.000e+00	0.00588	0.837	0.946
sns_000_01610	Al ₅ Yb ₈	13	-2.021	-2.413	0.000e+00	0.00424	0.458	1.194
sns_000_01632	Dy ₁₁ InRe ₃	15	-5.754	-5.91	-2.000e-06	0.0056	0.397	0.629
sns_000_01664	Dy ₄ Ga ₈ Pd ₄	16	-4.29	-4.471	0.000e+00	0.00823	0.343	0.527

Table S9. The profile of generated materials with Snub square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sns_000_01667	CsSnSrTlYb ₄	8	-1.666	-1.97	-7.000e-06	0.00363	0.968	1.686
sns_000_01679	Al ₆ Cd ₂ HfSn ₂ Tb ₂ Y	16	-4.117	-4.453	-7.000e-06	0.00555	0.75	1.727
sns_000_01697	AlGeHfMn ₆ Rh ₅ Zn	15	-7.188	-7.404	-1.000e-05	0.00944	0.416	1.243
sns_000_01698	CuGaMn ₄ Zn ₄ Zr ₃	13	-5.264	-5.602	0.000e+00	0.00386	0.892	1.638
sns_000_01700	Gd ₈ Ge ₆ Sb	15	-5.043	-5.22	-1.000e-06	0.00581	0.736	2.104
sns_000_01713	MnNi ₃ Ru ₆ Si ₂ Ti ₄	16	-7.799	-8.035	-2.000e-05	0.0039	0.376	1.044
sns_000_01721	Co ₄ Rh ₂ Sn ₇ U	14	-5.251	-5.707	-3.000e-06	0.00549	1.453	1.94
sns_000_01736	Al ₆ CaDy ₄ Li ₂	13	-3.57	-3.762	-4.000e-06	0.00782	0.447	0.613
sns_000_01759	Gd ₆ Pd ₉	15	-5.494	-5.637	0.000e+00	0.00623	0.41	0.972
sns_000_01771	GeLa ₃ Pt ₃ Rh ₃ Yb ₅	15	-5.069	-5.248	2.000e-06	0.00786	0.641	1.297
sns_000_01781	Co ₅ FeGeNi ₉	16	-5.831	-6.0	-4.000e-06	0.00671	0.417	0.599
sns_000_01807	Al ₅ FeRu ₈ Y ₂	16	-7.208	-7.423	0.000e+00	0.00416	0.42	0.692
sns_000_01811	Ca ₂ CdDy ₄ P ₅	12	-4.592	-5.353	-1.000e-06	0.00344	1.307	3.256
sns_000_01836	GaPd ₁₀ Yb ₄	15	-4.301	-4.761	-1.000e-06	0.00492	0.956	1.933
sns_000_01840	Al ₆ Ge ₂ Pd ₃ Tb ₄	15	-4.608	-4.891	0.000e+00	0.00682	0.399	1.501
sns_000_01863	Al ₆ Gd ₉	15	-4.393	-4.455	-5.800e-05	0.004	0.485	0.957
sns_000_01865	NiRu ₅ Si ₃ Sn ₂ UY	13	-7.133	-7.48	-7.000e-06	0.00617	0.711	2.27
sns_000_01867	Ru ₇ Sb ₂ Ti ₇	16	-7.831	-8.499	0.000e+00	0.00284	0.891	1.704
sns_000_01872	AgSb ₃ Yb ₁₀	14	-2.571	-2.649	0.000e+00	0.0027	0.869	1.103
sns_000_01879	CeFeGe ₈ Tb ₅	15	-5.215	-5.474	1.000e-05	0.004	1.197	1.043
sns_000_01887	Dy ₅ SbTl ₂	8	-3.806	-4.306	1.000e-06	0.00332	1.408	1.7
sns_000_01888	Dy ₄ Ga ₁₀	14	-3.432	-3.612	-4.000e-06	0.008	0.348	0.457
sns_000_01894	Au ₂ Ga ₄ GeNd ₇	14	-4.241	-4.529	-2.000e-06	0.00488	1.196	2.151
sns_000_01904	CdCoDy ₅ NaS ₈	16	-5.055	-5.587	-2.000e-06	0.0077	0.952	2.054
sns_000_01911	As ₂ Br ₃ Nd ₄ Rb	10	-3.501	-4.473	0.000e+00	0.005	1.322	2.165
sns_000_01944	Fe ₄ Th ₂	6	-7.67	-7.764	1.000e-06	0.0066	0.546	0.516
sns_000_01954	Ga ₄ Nd ₆ Os ₄ Rh ₂	16	-6.133	-6.315	0.000e+00	0.00869	0.458	1.75
sns_000_01968	Gd ₈ Pd ₆	14	-5.449	-5.521	1.000e-05	0.00832	0.097	0.732
sns_000_01972	Gd ₈ Pd ₄ Zn	13	-4.921	-5.023	-5.000e-06	0.00513	0.228	0.244
sns_000_01977	Ge ₅ Ru ₁₀	15	-6.915	-7.565	0.000e+00	0.00775	0.695	0.906
sns_000_02005	B ₄ Ru ₁₀ Si ₂	16	-8.071	-8.376	-1.000e-05	0.00396	0.333	1.061
sns_000_02019	AuNd ₄ OsRbSn ₆	13	-4.408	-4.76	1.000e-06	0.00701	1.283	3.341
sns_000_02030	Ga ₅ Nd ₆ PdRh	13	-4.652	-4.774	3.000e-06	0.00627	0.764	1.784
sns_000_02047	Al ₂ Au ₃ GeRu ₅ Si	12	-5.83	-6.173	-3.000e-06	0.00614	0.221	0.612
sns_000_02048	Fe ₂ Ni ₁₁ Si ₂ V	16	-6.13	-6.219	-1.500e-05	0.00874	0.139	0.263
sns_000_02054	Fe ₄ La ₂	6	-6.611	-6.813	1.000e-06	0.00551	0.822	2.2
sns_000_02060	RhSn ₆ Yb ₇	14	-3.284	-3.429	0.000e+00	0.00393	0.593	1.313
sns_000_02068	Ce ₃ Dy ₅ HoRuSi ₅	15	-5.783	-5.957	7.000e-06	0.00914	0.732	1.118
sns_000_02139	Ba ₃ Cl ₅ Co ₄ Mn	13	-4.425	-4.782	2.000e-06	0.00636	1.536	2.931
sns_000_02141	Cd ₂ Gd ₆ Tb ₆ Tl	15	-3.796	-3.981	5.000e-06	0.00543	0.773	0.962
sns_000_02150	Ga ₉ Gd ₇	16	-3.861	-4.036	-2.000e-06	0.00926	0.619	1.148
sns_000_02158	AgDy ₈ Mg ₂ Zn ₃	14	-3.277	-3.354	-5.000e-06	0.00285	0.287	0.32
sns_000_02173	Co ₂ Dy ₈ Si ₅	15	-5.388	-5.636	4.000e-06	0.00759	0.494	2.059
sns_000_02175	Ge ₂ Ni ₁₀	12	-5.293	-5.448	1.000e-06	0.00695	0.393	0.571
sns_000_02193	Co ₇ Gd ₄ Ge ₄	15	-5.443	-6.009	-4.000e-06	0.00711	1.341	3.213
sns_000_02196	Cd ₁₁ Nd ₄	15	-1.872	-2.023	1.000e-06	0.00808	0.418	0.589
sns_000_02219	Nd ₅ SnTl ₂	8	-3.8	-4.362	-1.000e-06	0.00341	0.804	2.193
sns_000_02225	Nd ₈ Rh ₄ Sn ₄	16	-5.666	-5.826	6.000e-06	0.0023	0.913	1.056
sns_000_02239	Ag ₂ Ga ₈ Nd ₅	15	-3.654	-3.868	2.000e-06	0.00488	0.515	0.685
sns_000_02244	AuGaMoP ₂ Ru ₄	9	-6.773	-7.109	1.000e-06	0.00814	0.223	0.407
sns_000_02254	Mg ₃ Ni ₆ Tb ₇	16	-4.445	-4.549	0.000e+00	0.00508	0.531	1.269
sns_000_02258	CuGa ₉ Gd ₆	16	-3.818	-4.167	-1.000e-06	0.00438	0.844	1.581

Table S9. The profile of generated materials with Snub square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sns_000_02265	Br ₄ Ru ₄	8	-4.731	-5.148	-3.000e-06	0.00888	0.778	1.002
sns_000_02275	Al ₇ Li ₃ Tb ₅	15	-3.691	-3.925	-3.000e-06	0.00863	0.152	1.886
sns_000_02318	Fe ₂ Ga ₅ Ni ₄ Ru ₅	16	-6.125	-6.171	-3.000e-06	0.00596	0.177	0.218
sns_000_02330	Ge ₃ LiNd ₈ Ni ₃	15	-4.599	-4.975	-7.000e-06	0.00859	0.546	1.596
sns_000_02335	CaDy ₅ Ga ₇ La ₂	15	-4.011	-4.162	0.000e+00	0.00561	0.085	0.287
sns_000_02337	Fe ₇ Ga ₉	16	-5.073	-5.231	1.000e-06	0.00853	1.084	1.192
sns_000_02340	Ga ₅ Ni ₄ U	10	-4.759	-4.807	-3.300e-05	0.00853	0.446	1.439
sns_000_02343	GePd ₂ RhRu ₄	8	-7.108	-7.305	-1.000e-06	0.00522	0.675	0.921
sns_000_02348	Dy ₆ Ga ₈ Ni ₂	16	-4.137	-4.288	-1.000e-05	0.00771	0.25	0.855
sns_000_02364	Ga ₇ MnNdSnTb ₅	15	-4.066	-4.434	-3.000e-06	0.00289	1.158	1.342
sns_000_02369	Na ₇ Yb ₉	16	-1.239	-1.317	0.000e+00	0.00405	1.517	1.54
sns_000_02373	Ir ₄ La ₂ Yb ₆ Zn ₃	15	-4.185	-4.286	-1.000e-06	0.00483	0.632	0.995
sns_000_02404	Ge ₃ InYb ₉	13	-2.797	-2.649	-1.000e-06	0.00575	0.2	0.331
sns_000_02427	Ni ₂ Sn ₅ Tb ₉	16	-4.747	-4.941	0.000e+00	0.00885	0.535	1.623
sns_000_02428	Sn ₈ Yb ₈	16	-3.161	-3.349	-1.000e-06	0.00282	0.603	0.645
sns_000_02442	Dy ₁₀ Fe ₂ Si ₄	16	-5.485	-5.653	-1.300e-05	0.00553	0.523	0.357
sns_000_02443	Sn ₉ Tb ₅ Y	15	-4.07	-4.808	-7.000e-06	0.00397	1.371	1.808
sns_000_02449	Ru ₄ Sr ₂	6	-5.466	-6.159	-3.400e-05	0.00605	0.552	0.527
sns_000_02453	Al ₂ Fe ₆ SiTi ₂	11	-6.934	-7.263	1.000e-06	0.00721	0.401	0.807
sns_000_02482	AlSn ₃ Yb ₈	12	-2.606	-2.659	-4.000e-06	0.00284	0.29	0.454
sns_000_02492	GeNd ₈ Tl ₅	14	-3.919	-4.116	0.000e+00	0.00601	0.3	0.308
sns_000_02497	Rh ₂ Tb ₈	10	-5.168	-5.445	0.000e+00	0.0058	0.842	2.242
sns_000_02508	FeNi ₂ P ₄ Ru ₆ Si ₃	16	-6.88	-7.36	-1.000e-05	0.00517	0.487	1.446
sns_000_02543	Ga ₉ Nd ₇	16	-3.892	-4.186	2.000e-06	0.00618	1.282	1.547
sns_000_02561	Cu ₂ Dy ₇ Ga ₅	14	-4.045	-4.23	-4.000e-06	0.00347	0.699	1.289
sns_000_02576	Si ₅ Tb ₁₀	15	-5.098	-5.365	-3.000e-06	0.00404	0.542	0.446
sns_000_02588	CoNd ₁₂ Ru ₂	15	-5.465	-5.514	-2.000e-06	0.00576	0.329	0.366
sns_000_02589	Al ₁₁ Ru ₅	16	-5.489	-5.819	0.000e+00	0.00445	0.847	1.121
sns_000_02590	Co ₂ Nd ₉ SmTb ₄	16	-4.826	-4.946	7.000e-06	0.00454	1.034	1.668
sns_000_02611	AlCo ₃ Tb ₇ Tc ₃	14	-6.044	-6.335	-4.000e-06	0.00596	0.852	1.042
sns_000_02617	AlCoMn ₅ Si ₄ U ₄	15	-4.92	-8.312	0.000e+00	0.00596	0.515	2.054
sns_000_02627	Ce ₄ Ga ₈ Nd ₄	16	-4.426	-4.617	2.000e-06	0.00339	0.944	0.967
sns_000_02631	Gd ₇ Ge ₈	15	-4.841	-5.293	1.000e-06	0.00275	0.708	1.431
sns_000_02632	Dy ₈ In ₂ Pb ₆	16	-4.496	-4.362	-1.000e-06	0.0037	0.453	0.608
sns_000_02651	AlCd ₅ Dy ₅ NbTl ₄	16	-3.061	-3.17	0.000e+00	0.00318	0.383	2.072
sns_000_02671	CdCoDy ₄ Ga ₅ TiU	13	-4.374	-4.818	-1.000e-06	0.00385	0.506	1.714
sns_000_02675	Ga ₂ GeRh ₅ Tb ₆	14	-5.686	-5.909	-4.000e-06	0.00393	0.956	1.513
sns_000_02687	Ge ₅ Yb ₁₀	15	-3.035	-3.073	-1.100e-05	0.00275	0.176	0.27
sns_000_02690	AgGa ₂ LaRu ₄ Sn ₂	10	-5.744	-5.841	-1.000e-06	0.009	0.295	0.369
sns_000_02693	Al ₃ GdLi ₃ Mn ₄	11	-4.564	-5.236	-1.000e-06	0.00613	1.767	1.758
sns_000_02716	Cd ₃ Ga ₅ Nd ₇	15	-3.588	-3.725	-3.000e-06	0.00432	0.358	0.683
sns_000_02742	Cd ₂ Dy ₄ Pd ₉	15	-4.933	-5.106	-3.900e-05	0.00923	1.313	1.601
sns_000_02778	Mg ₂ Pd ₅ SnYb ₇	15	-3.366	-3.46	-1.000e-06	0.00418	0.449	0.594
sns_000_02791	Gd ₆ Sn ₈	14	-4.338	-4.689	-6.000e-06	0.00324	0.913	1.203
sns_000_02795	Ga ₇ Pd ₅ Tb ₄	16	-4.357	-4.762	-1.900e-05	0.00654	1.164	2.072
sns_000_02800	CeDy ₅ Ga ₇ GeSb ₂	16	-3.969	-4.429	0.000e+00	0.00363	0.432	1.952
sns_000_02809	GePd ₈ SbYb ₆	16	-4.316	-4.491	-1.000e-06	0.00585	0.602	0.787
sns_000_02812	Ge ₂ In ₈ Nd ₅ Re	16	-4.085	-4.315	-8.000e-06	0.00851	0.599	1.537
sns_000_02832	Ga ₁₀ Tb ₆	16	-3.731	-3.992	-4.000e-06	0.00388	0.679	1.233
sns_000_02837	CdDy ₄ Ga ₁₁	16	-3.322	-3.484	2.000e-06	0.00451	0.406	0.473
sns_000_02846	Fe ₄ Pt ₁₂	16	-6.263	-6.603	-1.000e-04	0.00546	0.65	1.802
sns_000_02877	La ₂ Ni ₄	6	-5.335	-5.485	-1.390e-04	0.00866	0.527	0.775

Table S9. The profile of generated materials with Snub square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sns_000_02882	Dy ₄ Ga ₄ Ni ₂ Yb ₆	16	-3.187	-3.273	3.000e-06	0.00609	0.625	0.655
sns_000_02895	Dy ₈ Tl ₈	16	-3.64	-3.726	-2.000e-06	0.00751	0.553	0.662
sns_000_02927	ErInMg ₂ Nd ₅ Sn ₇	16	-3.984	-4.359	-2.000e-06	0.00479	0.938	1.939
sns_000_02931	Co ₃ Ga ₈ Gd ₄	15	-4.173	-4.499	-1.400e-05	0.00571	0.589	1.563
sns_000_02932	NiP ₈ Ru ₄ Ti ₃	16	-6.817	-7.318	0.000e+00	0.00832	0.52	1.879
sns_000_02946	FeNi ₁₀ Ti	12	-5.779	-5.954	1.000e-05	0.00666	0.276	0.419
sns_000_02953	Gd ₁₀ Ge ₃ Rh ₃	16	-5.725	-5.773	2.000e-06	0.00763	0.304	0.292
sns_000_02990	Ga ₅ Na ₄ PrSn	12	-3.958	-4.043	0.000e+00	0.00868	0.268	0.304
sns_000_03018	Al ₂ Ca ₂ Co ₄	8	-4.667	-4.871	6.000e-06	0.0083	0.412	0.891
sns_000_03028	SnTb ₈ Tl ₇	16	-3.747	-3.906	0.000e+00	0.00272	0.369	0.432
sns_000_03039	Ga ₁₂ Nd ₄	16	-3.472	-3.824	0.000e+00	0.00725	1.555	3.346
sns_000_03046	Ba ₄ Dy ₄ O ₈	16	-6.38	-6.847	0.000e+00	0.00482	0.485	2.404
sns_000_03095	Al ₆ Dy ₆ Ir	13	-4.577	-4.889	-1.000e-06	0.00358	0.772	1.629
sns_000_03096	AlAuCd ₄ GeNi ₆ Sb ₂ Y	16	-3.778	-4.012	-3.200e-05	0.00827	0.619	1.019
sns_000_03108	RuSi ₆ Tb ₇	14	-5.531	-5.747	-2.000e-06	0.00359	0.153	0.806
sns_000_03128	Al ₅ Gd ₆ GePd	13	-4.375	-4.697	-2.000e-06	0.00365	0.849	1.455
sns_000_03152	Co ₁₀ Ni ₄ Ti ₂	16	-6.593	-6.738	-1.000e-05	0.00891	0.382	1.228
sns_000_03155	Gd ₈ GeSn ₆	15	-4.701	-4.899	0.000e+00	0.00472	1.116	0.995
sns_000_03170	Rh ₃ Sn ₄ Yb ₄	11	-4.137	-4.486	-3.000e-06	0.00377	0.972	1.438
sns_000_03178	Ge ₆ Ni ₁₀	16	-5.236	-5.325	0.000e+00	0.00751	0.312	0.711
sns_000_03180	Co ₄ Dy ₇ Ga ₃	14	-4.824	-5.192	3.000e-06	0.0063	1.016	1.757
sns_000_03181	Al ₉ Yb ₆	15	-2.818	-2.979	0.000e+00	0.00211	0.391	2.313
sns_000_03188	Cd ₂ CuGa ₅ Ge ₄ Yb ₄	16	-2.879	-3.099	-4.000e-06	0.0076	1.055	1.553
sns_000_03242	Ge ₅ Pr ₂ Yb ₈	15	-3.404	-3.452	0.000e+00	0.00418	0.293	0.203
sns_000_03248	Al ₈ CoTb ₇	16	-4.412	-4.575	-2.000e-06	0.00289	0.3	0.96
sns_000_03255	Co ₁₀ P ₂ Si ₂	14	-6.656	-6.798	-3.000e-06	0.00942	0.243	0.328
sns_000_03261	Al ₂ Mn ₆ Sr ₂	10	-5.815	-6.212	-4.700e-05	0.00972	1.099	1.603
sns_000_03279	Dy ₈ Pt ₄ Sn ₂	14	-5.747	-5.77	-1.000e-06	0.00723	0.371	0.401
sns_000_03290	Ga ₆ MnNd ₉	16	-4.56	-4.619	0.000e+00	0.00433	0.292	1.237
sns_000_03315	CoGd ₄ La ₆ Sn ₂	13	-4.875	-5.073	1.000e-06	0.00714	0.435	1.147
sns_000_03328	Al ₇ CoDy ₅	13	-4.201	-4.563	1.000e-06	0.00669	0.97	1.463
sns_000_03340	Ga ₄ Nd ₁₀ Ni ₂	16	-4.502	-4.662	-2.000e-06	0.00579	0.686	1.707
sns_000_03357	Ga ₆ Mn ₁₀	16	-6.464	-6.615	0.000e+00	0.0055	0.224	1.784
sns_000_03386	Pt ₇ Ru ₉	16	-7.603	-7.802	-1.000e-05	0.00476	0.283	1.908
sns_000_03392	Al ₈ RhTb ₅	14	-4.434	-4.625	7.000e-06	0.00569	0.775	1.496
sns_000_03393	Nd ₄ RuSn ₁₀	15	-4.263	-4.783	1.000e-06	0.00509	0.879	1.461
sns_000_03399	Ru ₄ Th ₂	6	-8.433	-8.718	2.000e-06	0.00757	0.352	0.294
sns_000_03408	Nd ₇ Rh ₃ SnTiU	13	-5.711	-5.867	2.000e-06	0.00796	0.445	1.577
sns_000_03412	CaCo ₄ Dy ₈ Sr	14	-4.709	-4.825	-2.000e-05	0.00683	0.293	0.536
sns_000_03413	CaCd ₂ Os ₄ SnYb ₇	15	-3.922	-4.204	0.000e+00	0.00423	0.818	1.389
sns_000_03414	Tb ₅ Tl ₃	8	-3.441	-3.934	-1.000e-06	0.00364	1.467	1.05
sns_000_03425	Al ₂ Ru ₆	8	-7.793	-7.941	-1.000e-06	0.00352	0.081	0.145
sns_000_03426	Al ₇ Ru ₄ Si ₂	13	-5.676	-6.138	1.000e-06	0.00398	0.803	1.822
sns_000_03438	Ga ₃ RhSn ₂ Yb ₈	14	-2.931	-3.019	-1.000e-06	0.00337	0.278	0.927
sns_000_03445	Rh ₃ SnTb ₇	11	-5.461	-5.744	-3.000e-06	0.00769	0.993	0.907
sns_000_03447	Gd ₈ Ni ₄ Si ₄	16	-5.455	-5.632	1.600e-05	0.00744	0.382	0.951
sns_000_03464	Al ₁₀ LaTb ₅	16	-4.118	-4.476	0.000e+00	0.00332	1.021	1.841
sns_000_03474	Ga ₉ Nd ₇	16	-4.082	-4.233	-1.000e-06	0.00691	0.37	2.797
sns_000_03480	LaNd ₇ Tl ₈	16	-3.58	-3.897	0.000e+00	0.00397	0.713	0.752
sns_000_03488	Ni ₂ Sn ₃ Tb ₅	10	-4.726	-4.987	0.000e+00	0.00352	0.548	1.232
sns_000_03502	Hf ₅ Mn ₂ Ru ₅ Si	13	-9.104	-9.443	0.000e+00	0.00894	0.842	1.264
sns_000_03524	Dy ₆ Ga ₆ Ru ₄	16	-5.315	-5.504	-1.000e-06	0.00765	0.693	1.224

Table S9. The profile of generated materials with Snub square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sns_000_03527	BiCdEuGeNi ₂ Tb ₅	11	-4.142	-4.507	0.000e+00	0.00918	1.302	2.219
sns_000_03534	Co ₇ Gd ₅ La ₃	15	-5.579	-5.834	-2.000e-06	0.00931	0.631	2.065
sns_000_03541	Ga ₅ Nd ₈	13	-4.113	-4.389	3.000e-06	0.00523	1.003	2.488
sns_000_03574	Co ₂ Cu ₂ Ga ₃ Gd ₇ Pd ₂	16	-4.824	-4.978	-1.700e-05	0.00655	1.121	1.94
sns_000_03589	Co ₅ Ge ₄ La ₂	11	-5.834	-5.948	-1.000e-06	0.00616	0.42	0.973
sns_000_03600	Al ₅ Gd ₉	14	-4.297	-4.468	0.000e+00	0.00392	0.716	1.375
sns_000_03647	AuGa ₆ PdTb ₆	14	-4.177	-4.385	-1.500e-05	0.00978	0.69	1.545
sns_000_03651	Ga ₆ Gd ₇ W ₃	16	-5.455	-5.67	-8.000e-06	0.00615	0.227	0.403
sns_000_03664	Ga ₄ Li ₄ Mn ₇	15	-5.078	-5.325	-1.000e-06	0.0048	0.745	0.94
sns_000_03665	Ga ₇ Tb ₈	15	-4.187	-4.275	0.000e+00	0.00693	0.429	0.471
sns_000_03704	Al ₃ Ce ₂ Ge ₆ Tb ₄	15	-4.776	-5.037	-1.400e-05	0.00488	1.043	1.303
sns_000_03718	Pt ₄ Rh ₃ Sb ₂ Tb ₄	13	-5.964	-6.439	0.000e+00	0.00285	0.782	2.397
sns_000_03735	GeMgPt ₆ Tb ₈	16	-5.853	-5.992	0.000e+00	0.00576	0.361	1.389
sns_000_03749	Ge ₄ Nd ₈ NiRu ₃	16	-5.722	-5.935	4.000e-06	0.00487	0.718	1.591
sns_000_03767	Al ₈ CoDy ₄ Na	14	-3.927	-4.151	-2.000e-06	0.00733	0.726	1.525
sns_000_03787	Cd ₂ Ga ₅ Nd ₈	15	-3.903	-3.986	0.000e+00	0.00351	0.735	1.123
sns_000_03795	GaNd ₅ Pd ₄ Sn ₃	13	-4.784	-5.181	-2.000e-06	0.00611	1.086	2.065
sns_000_03800	Rh ₄ Sn ₂ Tb ₆ V	13	-5.856	-6.105	-4.000e-06	0.00767	0.345	0.965
sns_000_03802	Al ₈ CaRu ₅	14	-5.692	-5.903	0.000e+00	0.00479	0.726	1.156
sns_000_03810	AlCdGa ₅ Sc ₃ Yb ₅	15	-3.114	-3.271	-2.000e-06	0.0072	0.519	0.808
sns_000_03815	AgGd ₄ Ge ₄ Rh ₅ Zr	15	-5.864	-6.17	-2.000e-06	0.00731	0.446	1.683
sns_000_03832	Ga ₇ GeYb ₇	15	-2.569	-2.851	-9.000e-06	0.00579	0.561	1.949
sns_000_03857	Ir ₃ Se ₈ Tb ₄	15	-5.411	-5.817	-2.000e-06	0.00563	0.958	2.019
sns_000_03881	LiNd ₅ Ni ₆ SbSiSn	15	-4.966	-5.183	2.000e-06	0.00348	1.411	2.52
sns_000_03926	Co ₅ Tb ₈	13	-5.288	-5.581	-2.470e-04	0.00975	0.625	2.438
sns_000_03932	Al ₂ Ni ₁₄	16	-5.325	-5.445	-7.800e-05	0.0075	0.326	1.25
sns_000_03949	GeRu ₆ Si ₂ Tb ₅	14	-6.648	-6.922	-1.000e-06	0.0058	0.3	0.775
sns_000_03967	Dy ₄ RhScSn ₃ Sr	10	-4.449	-4.915	1.000e-06	0.00739	1.546	3.36
sns_000_03973	Al ₂ Au ₄ Ru ₄ Yb ₂ Zn ₂	14	-4.179	-4.634	2.000e-06	0.00497	1.722	1.978
sns_000_04003	Ga ₈ Tb ₈	16	-4.174	-4.362	0.000e+00	0.0064	0.591	0.979
sns_000_04010	Mn ₄ Sn ₂	6	-6.273	-6.881	0.000e+00	0.00862	0.512	0.766
sns_000_04032	Ga ₅ Nd ₆	11	-3.983	-4.278	6.000e-06	0.00804	1.492	1.983
sns_000_04065	Co ₄ Pr ₂	6	-5.845	-6.152	-8.000e-06	0.00766	0.819	2.744
sns_000_04092	CdLaPd ₆ Tb ₅	13	-4.973	-5.252	6.000e-06	0.00413	0.642	1.272
sns_000_04130	AlFe ₇	8	-7.173	-7.584	-5.000e-06	0.00904	0.319	0.983
sns_000_04135	Ga ₇ Mg ₂ Nd ₆	15	-3.674	-3.876	-3.000e-06	0.0067	0.217	0.826
sns_000_04140	NdP ₃ Ru ₄	8	-7.255	-7.517	2.000e-06	0.00704	0.148	1.028
sns_000_04147	FeNb ₂ Ru ₈ SiTiZn ₃	16	-7.457	-7.693	0.000e+00	0.00649	0.296	1.458
sns_000_04148	CoGd ₈ Si ₆	15	-5.393	-5.582	1.200e-05	0.00926	0.331	1.732
sns_000_04182	Co ₂ Ga ₁₀ Nd ₄	16	-3.985	-4.182	-2.000e-06	0.00974	0.516	0.645
sns_000_04198	Al ₅ Mn ₈ NiTcV	16	-7.065	-7.285	0.000e+00	0.00811	0.689	2.715
sns_000_04211	Ga ₈ HfRu ₆	15	-5.785	-6.062	-1.000e-06	0.00563	0.471	1.145
sns_000_04217	CoDy ₅ Ga ₈ OsW	16	-4.842	-5.14	2.000e-06	0.00748	0.723	1.09
sns_000_04227	Co ₂ Fe ₁₀ NbOsSi ₂	16	-7.87	-8.03	1.000e-05	0.00866	0.317	0.634
sns_000_04229	Al ₆ Dy ₆ Ti ₃	15	-4.573	-4.973	-4.000e-06	0.00402	0.642	1.812
sns_000_04234	GeMgPd ₃ Ru ₄ U	10	-6.269	-7.13	-1.500e-05	0.0087	1.147	3.384
sns_000_04237	Ge ₆ Yb ₁₀	16	-3.255	-3.29	0.000e+00	0.00225	0.189	0.243
sns_000_04251	Fe ₄ Se ₄	8	-5.846	-6.149	-3.000e-06	0.00794	0.345	1.023
sns_000_04263	CdNd ₈ NiSn ₆	16	-4.494	-4.733	-4.000e-06	0.00497	1.178	1.43
sns_000_04265	Ag ₂ Dy ₈ Ir ₂	12	-5.206	-5.37	-1.000e-06	0.00376	0.652	0.537
sns_000_04271	Ag ₂ Al ₃ Eu ₄ InNd ₄	14	-3.317	-3.489	0.000e+00	0.00496	0.199	0.383
sns_000_04273	Cd ₄ S ₈ Tb ₄	16	-4.236	-4.6	2.000e-06	0.0063	0.789	0.962

Table S9. The profile of generated materials with Snub square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sns_000_04275	Al ₂ Dy ₆ Ga ₈	16	-3.92	-4.115	0.000e+00	0.0081	0.466	1.436
sns_000_04280	Dy ₄ Sn ₂	6	-4.388	-4.793	0.000e+00	0.00468	0.961	1.387
sns_000_04293	Ga ₆ MoTb ₈ Tl	16	-4.486	-4.627	-1.000e-06	0.00485	0.827	1.432
sns_000_04313	Dy ₁₀ Rh ₅	15	-6.003	-6.04	0.000e+00	0.00838	0.363	0.806
sns_000_04317	Gd ₆ Li ₂ Si ₈	16	-4.857	-5.069	-8.000e-06	0.00653	0.572	1.085
sns_000_04324	CGeMn ₆ Ni ₅	13	-6.99	-7.246	-4.000e-06	0.00499	0.39	1.21
sns_000_04348	Al ₉ Gd ₆	15	-4.208	-4.323	1.000e-06	0.00313	0.343	2.324
sns_000_04367	Co ₃ Dy ₆ Ga ₇	16	-4.574	-4.687	0.000e+00	0.00564	0.433	0.494
sns_000_04387	Fe ₃ Ga ₄ GdP ₂ Ru ₄	14	-6.135	-6.576	-1.000e-06	0.00505	0.58	1.369
sns_000_04398	Ni ₁₁ TaV ₄	16	-6.692	-6.876	0.000e+00	0.00878	0.253	0.277
sns_000_04406	EuKNd ₄ Rh ₂ Sn ₂	10	-4.539	-4.756	-4.000e-06	0.00675	0.645	0.946
sns_000_04452	Dy ₈ Ga ₇	15	-4.049	-4.309	-9.000e-06	0.00441	0.39	1.959
sns_000_04468	Ge ₄ Tb ₄ V ₇	15	-6.401	-6.738	-1.000e-05	0.00766	0.647	1.146
sns_000_04470	Al ₆ GeYb ₇	14	-2.729	-2.875	-1.000e-06	0.0024	0.444	1.452
sns_000_04503	Al ₃ Ga ₃ Gd ₇	13	-4.212	-4.305	-4.000e-06	0.00465	0.611	1.083
sns_000_04532	Dy ₅ Ga ₆ MgNdSn ₂ Sr	16	-3.589	-3.801	-1.000e-06	0.00561	0.987	1.922
sns_000_04536	Ga ₈ Ru ₇	15	-5.951	-6.117	-1.000e-05	0.00957	0.622	1.673
sns_000_04543	Gd ₈ Si ₈	16	-5.256	-5.561	-1.000e-06	0.0051	0.55	0.759
sns_000_04565	Pd ₈ Tb ₇	15	-5.545	-5.632	-1.000e-06	0.00477	0.395	1.284
sns_000_04593	Ga ₄ Ru ₆ TiU	12	-7.017	-7.394	0.000e+00	0.00477	0.613	0.594
sns_000_04616	CaNaNd ₄ Rh ₄ Sb	11	-5.129	-5.424	-3.000e-06	0.00538	0.798	2.225
sns_000_04629	Ga ₁₂ Nd ₄	16	-3.409	-3.788	-1.000e-06	0.00524	1.206	1.68
sns_000_04641	Nd ₇ Rh ₃ Sn ₅	15	-5.268	-5.558	-2.000e-06	0.00375	0.687	1.371
sns_000_04660	Ge ₈ Nd ₈	16	-4.902	-5.213	0.000e+00	0.00711	0.815	0.536
sns_000_04663	Mn ₇ O ₈ Zn	16	-6.934	-7.445	1.000e-05	0.00777	0.862	1.951
sns_000_04669	Sn ₅ Yb ₁₀	15	-2.639	-2.769	-4.000e-06	0.00334	0.363	0.687
sns_000_04693	LaSnSrTb ₅	8	-4.05	-4.246	-2.000e-06	0.0024	0.83	1.08
sns_000_04698	CoDy ₈ Ga ₆	15	-4.354	-4.515	3.000e-06	0.00526	0.508	2.707
sns_000_04710	Nd ₈ Pt ₅ Sb ₂	15	-5.832	-6.003	-1.900e-05	0.0058	0.631	0.818
sns_000_04719	Ge ₆ Mn ₈ Ni ₂	16	-6.518	-6.744	0.000e+00	0.00704	0.476	0.546
sns_000_04722	Fe ₄ Ga ₂ NbNi ₈	15	-5.993	-6.151	-4.000e-06	0.00797	0.349	0.463
sns_000_04725	FeGa ₉ Mn ₅ Ti	16	-5.082	-5.44	-3.000e-06	0.00667	0.847	1.532
sns_000_04754	Sn ₈ Yb ₈	16	-3.169	-3.348	3.000e-06	0.00529	0.484	0.545
sns_000_04761	Ga ₄ GeNd ₇ Si ₄	16	-4.72	-4.909	-2.000e-06	0.0049	0.616	1.35
sns_000_04768	Pt ₄ Sn ₂ Tb ₉	15	-5.458	-5.644	1.000e-06	0.00701	0.717	0.77
sns_000_04769	CeGaTb ₅ Th	8	-4.748	-4.93	1.000e-06	0.00806	0.381	0.701
sns_000_04770	FeRu ₄ Si ₆ Ti ₅	16	-7.778	-7.975	-1.000e-05	0.00424	0.284	0.619
sns_000_04771	AlCo ₂ Dy ₈ Sb ₂	13	-4.826	-5.149	2.000e-06	0.00652	0.981	1.948
sns_000_04802	GeNi ₁₁	12	-5.279	-5.439	-1.000e-05	0.00696	0.281	1.182
sns_000_04822	Ga ₃ Gd ₈ Ni ₅	16	-4.832	-4.932	-7.000e-06	0.00845	0.398	1.417
sns_000_04831	Ga ₄ Tb ₄	8	-4.019	-4.321	2.000e-06	0.00646	0.545	0.77
sns_000_04842	AuBaDy ₄ Sn ₂ TeTl	10	-4.162	-4.137	-4.000e-06	0.00634	0.164	0.871
sns_000_04854	AlLiOs ₄ Tb ₁₀	16	-5.985	-6.2	0.000e+00	0.00526	0.749	0.772
sns_000_04859	GeRh ₆ Si ₂ Yb ₆	15	-4.891	-5.184	0.000e+00	0.0041	1.001	1.999
sns_000_04895	Cl ₇ CsGd ₆	14	-3.87	-4.23	-1.000e-06	0.00239	0.981	2.497
sns_000_04896	Ag ₃ Al ₆ Gd ₄	13	-3.651	-4.058	-1.000e-06	0.0045	0.78	1.177
sns_000_04900	Pt ₄ Sn ₂ SrYb ₅	12	-3.944	-4.219	-1.000e-06	0.00593	1.269	2.971
sns_000_04915	AlCaGa ₂ Nd ₄ Pd ₇	15	-4.92	-5.157	-1.100e-05	0.00752	0.877	1.978
sns_000_04918	Ni ₈ P ₂ ScSiVZr ₂	15	-6.293	-6.673	1.000e-05	0.00841	0.861	1.333
sns_000_04928	Ca ₂ P ₄ Ru ₄ Zn	11	-5.857	-6.235	1.000e-06	0.00353	0.469	1.923
sns_000_04929	Al ₂ Ni ₂ Sn ₄ Tb ₈	16	-4.684	-4.79	1.000e-06	0.00566	0.571	0.779
sns_000_04939	Ga ₆ La ₃ PdRu ₄	14	-5.478	-5.702	1.000e-06	0.00714	0.44	1.116

Table S9. The profile of generated materials with Snub square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sns_000_04951	CdDy ₈ Ga ₆ In	16	-4.126	-4.099	4.000e-06	0.00778	0.319	0.392
sns_000_04978	Gd ₇ Pd ₆	13	-5.449	-5.517	-2.000e-06	0.00454	0.342	0.874
sns_000_05004	Pd ₈ Yb ₈	16	-4.084	-4.184	-2.000e-06	0.00361	0.425	0.379
sns_000_05005	Ga ₈ Tb ₈	16	-4.025	-4.317	0.000e+00	0.00416	0.163	0.32
sns_000_05012	HfMnSi ₆ Ta ₂ Tb ₅	15	-6.712	-6.882	0.000e+00	0.00374	0.359	0.463
sns_000_05013	Al ₈ Dy ₄ Ni	13	-4.09	-4.501	-1.000e-06	0.00511	1.094	1.429
sns_000_05029	Ge ₂ NiRu ₈ Si	12	-7.597	-7.867	0.000e+00	0.00968	0.451	1.792
sns_000_05049	Fe ₂ Mn ₇ NiSi ₆	16	-7.379	-7.597	-5.000e-05	0.00501	0.701	0.929
sns_000_05058	Al ₁₁ LiTb ₄	16	-3.852	-4.105	2.000e-06	0.00446	0.59	1.534
sns_000_05108	Br ₄ Mn ₄	8	-4.809	-5.374	-1.000e-06	0.0058	1.19	2.276
sns_000_05130	Cd ₂ Ge ₂ Nd ₆ Sn ₂	12	-4.133	-4.288	-2.000e-06	0.00478	0.578	0.485
sns_000_05133	Nd ₈ Pt ₈	16	-6.431	-6.544	-1.000e-05	0.00585	0.213	0.68
sns_000_05139	FeP ₄ Ru ₉	14	-7.956	-8.269	0.000e+00	0.00676	0.841	0.677
sns_000_05145	IrLaPdSb ₂ Tb ₅ Zn ₄	14	-4.216	-4.423	-3.000e-06	0.00492	0.942	2.22
sns_000_05156	Co ₄ Ga ₅ Tb ₆	15	-4.72	-4.992	1.000e-05	0.00795	0.64	0.827
sns_000_05166	CdDy ₅ GaGdPd ₅	13	-4.897	-5.109	-1.000e-06	0.00635	1.198	1.669
sns_000_05184	Gd ₂ Ni ₄	6	-5.35	-5.406	-2.650e-04	0.00594	0.334	0.293
sns_000_05226	Pd ₃ Rh ₅ Yb ₈	16	-4.423	-4.596	-2.000e-06	0.0048	0.544	1.414
sns_000_05239	FeNd ₈ Si ₅	14	-5.366	-5.559	-2.000e-05	0.00384	0.661	2.341
sns_000_05254	CaGe ₅ Nd ₈ Tl	15	-4.807	-4.902	0.000e+00	0.00263	0.571	0.467
sns_000_05260	Al ₅ Gd ₆ Ge ₃ Mn ₂	16	-4.883	-5.232	0.000e+00	0.00444	0.573	0.55
sns_000_05271	Al ₅ Gd ₇ Ni	13	-4.45	-4.623	-8.600e-05	0.00483	0.976	2.306
sns_000_05280	Al ₃ Ge ₃ LaPrTb ₄	12	-4.55	-4.818	-2.000e-06	0.00729	0.394	1.323
sns_000_05288	Co ₅ GdGeNi ₆ SbSi	15	-5.69	-5.86	-2.000e-06	0.00712	0.178	0.946
sns_000_05299	Ce ₆ Ge ₃ Pd ₂ Tb ₄	15	-5.391	-5.582	0.000e+00	0.00324	0.721	1.547
sns_000_05310	BaCa ₄ CdGe ₂ Tl ₁ Yb ₅	14	-2.3	-2.401	0.000e+00	0.00418	0.656	0.622
sns_000_05325	Cu ₂ Dy ₇ Ga ₆	15	-3.939	-4.161	1.000e-06	0.00594	0.641	1.123
sns_000_05333	Ga ₃ Na ₂ Tb ₈	13	-3.565	-3.697	-4.000e-06	0.0079	0.423	0.453
sns_000_05341	Dy ₁₂ Os ₂	14	-5.486	-5.55	5.000e-06	0.009	0.208	0.23
sns_000_05378	Dy ₇ Pt ₆ Sn	14	-6.198	-6.184	-3.000e-06	0.00641	0.353	0.973
sns_000_05387	GeMn ₄ P ₅	10	-6.506	-6.947	-2.000e-06	0.0057	0.409	0.683
sns_000_05400	Tl ₂ Yb ₄	6	-1.595	-2.024	-4.000e-06	0.0023	0.692	1.388
sns_000_05423	Dy ₆ Ga ₈ GePt	16	-4.096	-4.379	-2.000e-06	0.00917	0.58	1.309
sns_000_05426	Ge ₅ Nd ₈ Zn ₂	15	-4.565	-4.741	-1.600e-05	0.00292	0.329	0.317
sns_000_05430	Dy ₇ La ₃ Sn ₆	16	-4.71	-4.836	0.000e+00	0.00492	0.536	1.906
sns_000_05433	Yb ₁₁ Zn ₄	15	-1.41	-1.474	-1.000e-06	0.00219	0.509	0.537
sns_000_05440	Li ₂ Ni ₃ Sn ₄ Tb ₄	13	-4.335	-4.493	2.000e-06	0.00767	0.284	0.984
sns_000_05454	Dy ₆ LaRh ₃ Si ₆	16	-5.789	-6.067	-2.000e-06	0.00714	0.694	1.941
sns_000_05457	KRu ₄ SSe ₄	10	-5.406	-5.772	0.000e+00	0.00768	0.955	0.779
sns_000_05462	FeNi ₁₁	12	-5.441	-5.615	7.000e-06	0.00695	0.382	0.991
sns_000_05485	Ni ₅ SbSn	7	-4.991	-5.128	-1.000e-06	0.00676	0.482	0.565
sns_000_05491	Ga ₃ Nd ₁₂	15	-4.34	-4.537	-3.000e-06	0.00376	1.305	1.38
sns_000_05497	Co ₂ NiP ₅ Ru ₄	12	-6.998	-7.223	7.000e-06	0.00888	0.628	0.603
sns_000_05503	Ga ₂ Gd ₆ Na ₄	12	-3.11	-3.171	-2.000e-06	0.00731	0.982	0.706
sns_000_05516	Al ₄ CaCd ₂ CeNd ₄	12	-3.549	-3.699	-1.000e-06	0.00559	0.612	0.47
sns_000_05521	AlDy ₄ Ga ₉ Ho ₂	16	-3.841	-4.107	-1.000e-06	0.00549	0.351	0.994
sns_000_05532	Sn ₇ Yb ₈	15	-2.897	-3.065	-1.200e-05	0.00605	0.888	1.87
sns_000_05534	Co ₂ Dy ₆ P ₈	16	-5.995	-6.236	0.000e+00	0.006	0.623	1.726
sns_000_05547	Nd ₄ Sn ₂ Tl ₂	8	-3.635	-4.372	-2.000e-06	0.00476	2.022	1.973
sns_000_05550	AlCd ₃ IrNd ₅ PrYb ₂	13	-3.64	-3.796	-7.000e-06	0.00596	1.107	1.997
sns_000_05554	Ge ₆ Ru ₅ Y ₂	13	-6.669	-6.975	5.000e-06	0.00731	0.584	0.652
sns_000_05559	Cs ₂ Tb ₄	6	-2.515	-2.762	-9.000e-06	0.00338	1.266	1.415

Table S9. The profile of generated materials with Snub square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sns_000_05565	Co ₄ EuGeTb ₆	12	-5.031	-5.288	-4.000e-06	0.0062	1.063	1.448
sns_000_05567	Al ₈ Tb ₇	15	-4.262	-4.379	0.000e+00	0.00582	0.582	1.298
sns_000_05591	Ba ₂ Cd ₃ Sb ₃ Tb ₈	16	-3.612	-3.772	-3.000e-06	0.00577	0.854	0.951
sns_000_05598	Fe ₅ Ga ₃ TmU	10	-5.91	-6.583	0.000e+00	0.00508	0.908	1.507
sns_000_05621	Al ₂ FeNi ₁₁ SbTi	16	-5.661	-5.805	-1.400e-05	0.00611	0.328	0.959
sns_000_05629	Mg ₂ Mn ₄	6	-5.341	-5.979	-1.500e-05	0.00948	0.727	0.642
sns_000_05642	Al ₄ Ge ₃ Nd ₇ PrV	16	-4.933	-5.058	-1.000e-06	0.00245	0.566	0.619
sns_000_05647	Ga ₈ Yb ₈	16	-2.43	-2.566	-2.200e-05	0.00365	0.91	1.874
sns_000_05648	Nd ₇ Ni ₅ Sb	13	-5.09	-5.228	-2.500e-05	0.0093	0.653	2.415
sns_000_05681	Al ₆ Dy ₇	13	-4.219	-4.453	0.000e+00	0.00644	0.412	2.06
sns_000_05710	AlCuFe ₂ Ga ₅ Mn ₅ Nb	15	-6.01	-6.224	-3.000e-06	0.00656	0.806	2.027
sns_000_05751	Ga ₉ Nd ₇	16	-4.001	-4.183	0.000e+00	0.00851	1.096	1.589
sns_000_05757	Co ₄ Ge ₂ Nd ₅ Sn ₃	14	-5.237	-5.441	0.000e+00	0.00685	0.378	0.558
sns_000_05768	AlNi ₁₄	15	-5.247	-5.332	5.000e-06	0.00553	0.08	0.169
sns_000_05781	Ce ₂ Se ₈ Yb ₄	14	-4.709	-4.984	-6.000e-06	0.00465	1.409	2.853
sns_000_05789	Ru ₈ Si ₃ W ₄	15	-9.01	-9.52	0.000e+00	0.00866	0.881	2.493
sns_000_05820	Gd ₉ Ge ₅ Li	15	-4.82	-5.007	-1.000e-06	0.00377	0.5	0.511
sns_000_05835	Mn ₄ Tl ₂	6	-5.52	-5.977	0.000e+00	0.00652	0.486	0.46
sns_000_05854	AlGeNi ₁₀	12	-5.284	-5.455	3.000e-06	0.00672	0.296	0.444
sns_000_05857	AlDy ₅ Ga ₉ Tb	16	-3.835	-4.052	0.000e+00	0.00754	0.691	2.122
sns_000_05880	Ga ₇ Mn ₅ Pd ₂ Pt ₂	16	-5.352	-5.597	-3.000e-06	0.00767	0.257	0.517
sns_000_05887	GeNPr ₂ Ru ₅	9	-7.366	-7.64	2.000e-06	0.00575	1.047	1.663
sns_000_05892	Al ₆ Gd ₅ Ni ₅	16	-4.776	-4.978	1.000e-06	0.00934	0.911	1.82
sns_000_05902	Gd ₇ PRh ₄	12	-5.963	-6.182	-2.000e-06	0.00496	0.765	0.499
sns_000_05905	Ga ₈ Gd ₇	15	-4.046	-4.207	-3.000e-06	0.00495	0.369	1.51
sns_000_05939	Co ₅ Ga ₄ Li ₂ Np	12	-4.961	-5.348	-4.000e-06	0.00779	1.046	1.467
sns_000_05941	Al ₁₀ GeMgTb ₄	16	-3.912	-4.061	-6.000e-06	0.00393	0.644	1.118
sns_000_05955	Cd ₄ NaNd ₆ Sb ₄	15	-3.62	-3.802	-3.000e-06	0.00453	0.621	0.432
sns_000_05965	ReRu ₅ Si ₆ Ti ₃ V	16	-8.136	-8.28	-1.000e-05	0.00411	0.389	1.118
sns_000_05967	Gd ₆ Ru ₂ Si ₈	16	-5.692	-6.088	0.000e+00	0.00701	1.152	3.18
sns_000_05974	Ca ₃ Sn ₇ Tb ₄	14	-3.943	-4.057	2.000e-06	0.0092	0.878	2.418
sns_000_06015	Ir ₄ Tb ₅ Y ₇	16	-6.933	-6.964	0.000e+00	0.00406	0.203	0.605
sns_000_06021	Au ₃ Ba ₂ Sn ₆ Tb ₄	15	-3.846	-4.194	2.000e-06	0.0059	0.767	1.733
sns_000_06024	Cd ₂ Dy ₄ FeGa ₇	14	-3.509	-3.803	-6.000e-06	0.00378	1.111	1.6
sns_000_06047	Gd ₇ Ge ₈ Rh	16	-5.21	-5.344	0.000e+00	0.0069	0.229	1.486
sns_000_06058	Dy ₆ Ga ₉ Ni	16	-4.016	-4.143	-1.000e-06	0.0081	0.507	1.133
sns_000_06074	GeRh ₇ Tb ₆	14	-6.256	-6.586	-2.000e-06	0.00508	0.972	2.072
sns_000_06096	CaDy ₄ GdSiTe ₇ Zn	15	-4.358	-4.598	-2.000e-06	0.00551	0.817	2.172
sns_000_06112	Co ₄ Ge ₃ SnTe ₄	12	-4.458	-4.81	-5.000e-06	0.0077	0.877	1.263
sns_000_06150	Gd ₄ GePt ₆ Si ₂ Ti ₂	15	-6.241	-6.526	-2.100e-05	0.00975	0.899	1.619
sns_000_06157	Ga ₈ Nd ₆ Pr ₂	16	-4.187	-4.366	-1.000e-06	0.00547	0.282	0.327
sns_000_06166	Nd ₈ V ₆	14	-6.06	-6.224	-2.000e-06	0.00708	0.555	0.975
sns_000_06192	Al ₆ La ₃ SbTb ₅	15	-4.418	-4.678	-1.000e-06	0.0068	0.27	0.812
sns_000_06195	Dy ₅ GdPd ₈ Sb	15	-5.482	-5.641	-1.500e-05	0.00533	0.203	1.51
sns_000_06199	Nd ₄ Sb ₂ Sn ₂	8	-4.424	-5.138	0.000e+00	0.00419	1.623	2.055
sns_000_06201	Ga ₉ NiRu ₄	14	-4.691	-4.957	-1.000e-06	0.00838	0.447	2.177
sns_000_06210	GaLaPd ₇ Ru ₅	14	-6.121	-6.467	-5.000e-06	0.00907	0.938	0.782
sns_000_06212	Ga ₄ GeYb ₁₀	15	-2.369	-2.454	0.000e+00	0.00231	0.242	0.257
sns_000_06214	Ga ₄ LiTb ₄ Zr ₆	15	-5.509	-5.733	0.000e+00	0.00427	0.759	1.132
sns_000_06229	LaNd ₈ SbSn ₂	12	-4.611	-4.874	-1.000e-06	0.00752	0.929	0.889
sns_000_06232	Fe ₄ Si ₆ Zr	11	-6.58	-6.969	-5.200e-05	0.00906	0.68	0.926
sns_000_06240	AlCu ₄ Tb ₄ Zr ₆	15	-5.724	-5.896	0.000e+00	0.0056	0.767	1.778

Table S9. The profile of generated materials with Snub square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sns_000_06244	Ru ₅ Tb ₁₀	15	-6.173	-6.287	3.000e-06	0.0082	0.368	0.331
sns_000_06250	Dy ₄ Na ₄	8	-2.454	-2.661	1.000e-06	0.00406	0.565	0.701
sns_000_06264	Ga ₈ OsRu ₆	15	-5.968	-6.025	-6.000e-06	0.00858	0.244	0.589
sns_000_06266	Al ₆ Dy ₄ Sn	11	-3.956	-4.462	1.000e-06	0.00372	1.01	1.099
sns_000_06277	Nd ₂ Ru ₄	6	-7.274	-7.608	-7.000e-06	0.00576	0.632	0.471
sns_000_06288	Al ₁₂ Yb ₄	16	-2.982	-3.307	0.000e+00	0.00328	0.675	1.072
sns_000_06322	Ga ₄ Ni ₄ Tb ₇	15	-4.656	-4.795	-5.000e-06	0.00704	0.462	0.56
sns_000_06327	Ga ₅ Nd ₈	13	-4.174	-4.349	-3.000e-06	0.00586	0.576	0.995
sns_000_06328	ErGdNd ₅ Sn	8	-4.48	-4.709	-3.000e-06	0.00506	0.791	0.754
sns_000_06352	Al ₆ Ni ₂ Ru ₄ Zr ₄	16	-6.621	-6.944	0.000e+00	0.00837	0.521	0.759
sns_000_06359	Ga ₅ Mg ₂ Ru ₄ Tl	12	-4.594	-4.761	-2.000e-06	0.00755	0.711	1.16
sns_000_06388	CaSn ₄ Sr ₂ Yb ₈	15	-2.325	-2.496	-6.000e-06	0.00475	0.611	1.531
sns_000_06393	CdGd ₅ Sn ₆ Sr ₂	14	-3.867	-4.084	-5.000e-06	0.00791	0.589	1.153
sns_000_06404	Ru ₄ Se ₄	8	-6.148	-6.591	0.000e+00	0.00723	0.271	0.431
sns_000_06411	Pd ₄ Yb ₈	12	-3.187	-3.34	0.000e+00	0.00234	0.71	1.454
sns_000_06446	Dy ₆ Ga ₃ GeNi ₂ Si ₄	16	-4.867	-5.05	-2.000e-06	0.00397	0.943	0.928
sns_000_06453	CoFe ₁₀ Ga ₅	16	-6.226	-6.372	0.000e+00	0.00393	1.043	1.481
sns_000_06473	As ₄ Fe ₇ PTiW ₂	15	-7.39	-7.65	-1.000e-05	0.00745	0.63	0.857
sns_000_06515	Gd ₇ Pd ₇	14	-5.466	-5.604	-4.000e-06	0.00526	0.71	1.297
sns_000_06534	CdGa ₈ Nd ₅ U	15	-4.089	-4.232	1.000e-06	0.00669	0.33	0.457
sns_000_06536	Cd ₂ Gd ₆ Si ₅	13	-4.507	-4.697	-3.100e-05	0.00941	0.68	1.555
sns_000_06551	CdDy ₄ Ga ₄ GeIr ₂ Os	13	-4.954	-5.367	-2.000e-06	0.00653	0.696	1.313
sns_000_06582	Tb ₄ Tl ₂	6	-3.561	-3.969	-1.000e-06	0.00322	0.89	0.701
sns_000_06631	Dy ₆ Ga ₈ Sr	15	-3.661	-3.947	-7.000e-06	0.00775	0.876	2.458
sns_000_06674	Cl ₂ Dy ₄ Rb ₂ S ₄	12	-4.853	-4.949	-3.000e-06	0.00329	0.369	1.493
sns_000_06678	CaDy ₅ Si ₉ Sm	16	-5.102	-5.294	0.000e+00	0.00295	0.486	0.837
sns_000_06687	Al ₄ Ce ₄ Ru ₅ SiSn	15	-6.406	-6.691	1.000e-05	0.00397	0.484	1.345
sns_000_06696	Dy ₄ I ₄ Pt ₂	10	-3.948	-4.487	-3.000e-06	0.00476	0.83	2.325
sns_000_06718	Pt ₄ SSe ₃ Tb ₄	12	-5.012	-5.942	-3.000e-06	0.00815	1.127	3.295
sns_000_06727	Rh ₄ Sn ₈ Tb ₄	16	-5.269	-5.422	-2.000e-06	0.00537	0.511	0.401
sns_000_06732	Al ₃ Gd ₅ PtSi ₆ Ti	16	-5.004	-5.538	0.000e+00	0.00635	1.041	2.663
sns_000_06761	NaNd ₄ Sn ₅ Tl	11	-3.924	-4.005	-9.000e-06	0.00799	0.564	0.565
sns_000_06775	GaIrLi ₂ Nd ₇ Si ₄	15	-4.846	-5.171	-5.000e-06	0.00923	1.463	2.631
sns_001_00002	Dy ₇ LiNi ₆ Sb	15	-4.943	-5.07	-3.000e-06	0.00771	0.251	1.084
sns_001_00016	AlGe ₇ Yb ₇ Zn	16	-3.202	-3.405	0.000e+00	0.00552	0.474	0.47
sns_001_00036	LiNi ₄ Ru ₄ Sn ₅	14	-5.517	-5.701	3.000e-06	0.00996	0.308	0.766
sns_001_00059	Nd ₆ NiP ₃ Si ₄ Ti	15	-5.62	-6.029	-1.900e-05	0.00407	0.73	1.655
sns_001_00078	CaMgSnSr ₄ TlYb ₈	16	-1.812	-1.846	-3.000e-06	0.00754	0.265	0.317
sns_001_00082	Ge ₂ Na ₂ Nd ₆	10	-3.907	-4.069	0.000e+00	0.00426	0.37	0.546
sns_001_00130	Cd ₃ GeNa ₂ Ru ₅ Si ₂	13	-4.665	-4.941	0.000e+00	0.0061	0.437	0.585
sns_001_00133	BaBr ₂ Nd ₄ Os ₂ SeSiSn	12	-4.902	-5.54	-6.000e-06	0.005	0.875	2.229
sns_001_00136	Co ₅ Ga ₂ Ge ₅	12	-4.749	-5.358	-3.000e-06	0.00765	0.984	1.852
sns_001_00140	P ₁₀ Ru ₅	15	-6.406	-6.85	0.000e+00	0.00469	0.751	1.179
sns_001_00151	Co ₄ Se ₄	8	-5.346	-5.415	1.000e-06	0.00803	0.233	0.196
sns_001_00162	Ga ₈ Nd ₈	16	-4.132	-4.329	0.000e+00	0.00614	1.009	1.535
sns_001_00177	Co ₄ HoNd	6	-5.91	-6.19	-9.000e-06	0.00819	0.342	0.683
sns_001_00189	Al ₅ Dy ₉ Fe	15	-4.508	-4.723	3.000e-06	0.00329	0.593	1.287
sns_001_00196	Ga ₈ Gd ₆ Y ₂	16	-4.384	-4.569	0.000e+00	0.00102	0.179	1.164
sns_001_00261	Cu ₂ Fe ₃ Ru ₄ Si ₂ Tb	12	-6.697	-7.04	-1.000e-06	0.00575	0.983	1.569
sns_001_00266	Pd ₃ PrRu ₄ Sr	9	-5.839	-6.428	-3.000e-06	0.0059	0.82	1.271
sns_001_00269	Gd ₆ PrSn ₆	13	-4.537	-4.814	-1.000e-06	0.00304	0.83	2.234
sns_001_00270	Ru ₈ Sb ₂ Si ₅	15	-7.016	-7.44	0.000e+00	0.00899	0.216	0.573

Table S9. The profile of generated materials with Snub square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sns_001_00286	Nd ₄ Tl ₁₁	15	-2.877	-3.035	-1.000e-06	0.00391	1.219	2.512
sns_001_00311	CaSn ₄ Sr ₆ Yb ₄	15	-2.331	-2.511	1.000e-06	0.00372	1.522	1.872
sns_001_00348	BGeP ₂ Ru ₇	11	-7.546	-7.937	-1.000e-06	0.00418	0.297	0.887
sns_001_00362	Cd ₅ GaMgYb ₈	15	-1.464	-1.648	1.000e-06	0.00408	0.522	2.059
sns_001_00413	Ga ₆ Nd ₁₀	16	-4.458	-4.485	4.000e-06	0.00551	0.212	0.288
sns_001_00420	Gd ₄ Ge ₃ Mn ₆ Pd ₂ Zn	16	-5.796	-6.034	2.000e-06	0.00547	0.348	0.787
sns_001_00422	Nd ₈ Rh ₂ Sn ₅	15	-5.168	-5.385	1.000e-06	0.00624	0.656	2.363
sns_001_00427	As ₂ Pt ₄ Tb ₁₀	16	-5.739	-5.962	1.000e-06	0.00276	0.94	0.729
sns_001_00432	Ga ₃ Tb ₈	11	-4.074	-4.411	-1.000e-06	0.00519	1.425	1.232
sns_001_00437	Pd ₂ Ru ₄ Sn ₁₀	16	-5.16	-5.41	-6.000e-06	0.00527	0.599	0.917
sns_001_00469	Ga ₁₀ Nd ₆	16	-3.829	-4.058	-2.000e-06	0.00456	0.532	2.011
sns_001_00471	Nd ₆ Si ₈	14	-5.215	-5.542	-9.000e-06	0.00587	0.484	1.027
sns_001_00475	Cd ₂ Ga ₈ Yb ₆	16	-2.376	-2.528	1.000e-06	0.00734	0.45	0.531
sns_001_00513	Dy ₆ Ga ₃ Ge ₅ Ru	15	-4.747	-5.08	-2.000e-06	0.00411	0.872	3.357
sns_001_00523	Co ₄ InLu	6	-5.485	-5.856	-1.000e-05	0.00672	0.395	0.904
sns_001_00544	Au ₂ Rh ₂ Sn ₂ Yb ₉	15	-3.207	-3.383	-8.000e-06	0.00478	0.339	1.153
sns_001_00569	Al ₆ Dy ₄ GeLaNa	13	-3.787	-4.154	-9.000e-06	0.00702	1.085	1.606
sns_001_00607	Al ₃ Ir ₂ Nd ₆ Si ₄	15	-5.501	-5.77	-3.400e-05	0.00939	0.65	1.199
sns_001_00612	Ga ₇ Nd ₆	13	-4.032	-4.161	-3.000e-06	0.00598	0.705	0.881
sns_001_00648	Er ₂ Ga ₆ MgNd ₆	15	-3.919	-4.118	3.000e-06	0.0077	0.397	1.695
sns_001_00652	Co ₄ NdSn ₅	10	-4.642	-5.172	-1.800e-05	0.00837	1.377	2.03
sns_001_00666	Dy ₄ GdScSi ₈	14	-5.237	-5.597	1.000e-06	0.00388	0.992	1.335
sns_001_00677	Ga ₅ Nd ₈	13	-4.24	-4.363	-1.000e-06	0.00488	0.099	0.425
sns_001_00681	CaNd ₅ Sb ₅ SnSrTl	14	-4.282	-4.724	-3.700e-05	0.00888	1.11	1.905
sns_001_00703	Nd ₇ S ₇	14	-5.868	-6.074	-6.000e-06	0.00425	0.088	0.821
sns_001_00739	Pd ₃ SnYb ₇	11	-3.035	-3.318	0.000e+00	0.00415	1.388	1.427
sns_001_00750	MnNiRu ₈ Si ₅ Ti	16	-7.925	-8.158	1.000e-05	0.00425	0.673	0.691
sns_001_00752	Cd ₄ Gd ₄ La ₄ Pd ₄	16	-4.148	-4.253	-2.000e-06	0.00893	0.402	1.45
sns_001_00816	CaGa ₇ Yb ₇	15	-2.454	-2.634	0.000e+00	0.00531	0.33	1.407
sns_001_00822	Pd ₅ Tb ₁₀	15	-5.261	-5.326	-1.800e-05	0.00441	0.623	1.181
sns_001_00826	Co ₃ GaSi ₂ Tb ₈	14	-5.264	-5.415	0.000e+00	0.00609	0.496	0.706
sns_001_00830	Gd ₅ Ru ₄ Sn ₃	12	-5.869	-6.149	-7.000e-06	0.00761	0.85	1.55
sns_001_00871	Ce ₄ Ru ₄ Sn ₈	16	-5.751	-6.012	-6.000e-06	0.00608	0.738	1.339
sns_001_00897	Mn ₄ Te ₂	6	-6.115	-6.594	-1.100e-05	0.00629	0.943	1.142
sns_001_00908	Ga ₃ Li ₆ Mn ₄ OsPdSb	16	-4.491	-4.784	-2.000e-06	0.0058	0.63	1.325
sns_001_00919	Nd ₁₀ Ni ₄	14	-4.969	-4.993	-8.000e-06	0.00729	0.11	0.166
sns_001_00924	Pd ₇ Yb ₈	15	-3.886	-4.035	-1.600e-05	0.00514	0.496	1.389
sns_001_00947	Au ₅ Dy ₅ LaPd ₃	14	-4.489	-4.933	-3.000e-06	0.00511	0.941	1.058
sns_001_00961	Al ₄ Gd ₆ Li ₃ Sb	14	-3.732	-4.024	-1.000e-06	0.00428	0.964	1.327
sns_001_00989	AlFe ₅ GaLa ₂ Ni ₂ P ₃	14	-6.216	-6.383	-1.000e-06	0.00492	0.691	0.978
sns_001_00997	Gd ₇ MnSe ₈	16	-5.51	-5.865	0.000e+00	0.00387	0.715	1.772
sns_001_00999	CrGeNi ₅ Sn	8	-5.389	-5.689	-1.000e-06	0.00741	1.007	1.751
sns_001_01034	Ga ₆ In ₂ Yb ₈	16	-2.73	-2.573	-2.000e-06	0.00458	0.052	0.064
sns_001_01042	Gd ₈ SbSi ₇	16	-5.24	-5.531	1.000e-06	0.00419	0.769	0.977
sns_001_01048	Ce ₃ PdRu ₄ Sn ₇	15	-5.737	-6.054	0.000e+00	0.0051	0.715	1.411
sns_001_01070	Co ₃ LiMg ₂ NbPRu ₈	16	-6.969	-7.165	0.000e+00	0.00936	0.162	0.965
sns_001_01096	GaNi ₉ P ₂ SiSn ₂	15	-4.996	-5.355	3.000e-06	0.00722	0.879	1.448
sns_001_01106	I ₄ Ni ₄	8	-2.956	-3.256	-2.100e-05	0.00803	1.609	2.509
sns_001_01115	NaSn ₂ SrYb ₈ Zn ₂	14	-2.028	-2.053	-1.000e-06	0.00626	0.205	0.233
sns_001_01166	Co ₄ Cs ₂	6	-3.845	-4.332	9.000e-06	0.00679	0.81	1.061
sns_001_01169	Al ₃ Ca ₃ Dy ₄ Rh ₄	14	-4.787	-5.099	-5.000e-06	0.00537	0.977	2.576
sns_001_01238	Gd ₈ MnRu ₂	11	-5.55	-5.862	-3.000e-06	0.008	1.17	2.931

Table S9. The profile of generated materials with Snub square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sns_001_01239	Al ₂ Gd ₆ Ni ₅	13	-4.902	-5.123	5.000e-06	0.00612	0.622	1.181
sns_001_01266	Na ₂ Nd ₆	8	-3.569	-3.683	-1.200e-05	0.00364	0.519	0.742
sns_001_01286	Mn ₄ P ₃ VW ₃ Zr ₄	15	-8.893	-9.171	-1.000e-05	0.00671	0.69	1.322
sns_001_01304	Gd ₆ Mn ₃ Si ₂ Sn ₂	13	-5.519	-5.602	-1.700e-05	0.00825	0.287	0.786
sns_001_01319	Dy ₄ Pb ₂	6	-4.269	-4.52	2.000e-06	0.00461	0.97	1.148
sns_001_01323	Gd ₆ Ge ₅ Rh ₅	16	-5.924	-6.091	-4.000e-06	0.00769	0.399	1.192
sns_001_01359	Ga ₆ Nd ₄ Os ₂ Sm ₂	14	-5.066	-5.143	-1.000e-06	0.00917	0.24	0.759
sns_001_01368	Ni ₄ Te ₂	6	-4.196	-4.647	-2.500e-05	0.00803	0.891	1.449
sns_001_01380	Dy ₆ Ga ₁₀	16	-3.8	-3.949	3.000e-06	0.00811	0.555	0.849
sns_001_01400	Cu ₇ Dy ₆ Ga ₂ Mn	16	-4.324	-4.398	0.000e+00	0.00558	0.225	0.402
sns_001_01406	Al ₄ Ge ₂ Hf ₂ Ru ₆	14	-7.058	-7.32	0.000e+00	0.00397	0.601	0.686
sns_001_01426	Ge ₄ Nd ₈ Ru ₂ Si ₂	16	-5.631	-5.856	-3.000e-06	0.00533	0.392	1.361
sns_001_01436	CuMn ₅ P ₈	14	-5.996	-6.765	-1.700e-05	0.00887	0.669	0.916
sns_001_01457	Ga ₃ Ir ₃ Nd ₈ Sn	15	-5.595	-5.669	1.000e-06	0.00373	0.329	0.338
sns_001_01466	AsFe ₂ HfNi ₈ Si ₂ Zn	15	-5.738	-5.987	-1.900e-05	0.00728	0.567	1.042
sns_001_01482	Nd ₇ Sb ₂ SnZn ₅	15	-3.509	-3.794	-2.000e-06	0.0055	1.434	3.01
sns_001_01553	NiRu ₆ Si ₈ W	16	-7.569	-7.793	0.000e+00	0.00441	1.176	2.769
sns_001_01554	Ga ₈ Nd ₈	16	-4.126	-4.371	-3.000e-06	0.00411	0.309	0.624
sns_001_01571	Pt ₄ Yb ₁₀	14	-3.557	-3.596	-2.000e-06	0.00442	0.195	0.148
sns_001_01589	Sb ₂ Tb ₄ TeTlW	9	-4.747	-5.442	0.000e+00	0.00295	1.399	1.696
sns_001_01608	AlGe ₃ Nd ₇ Ru ₄	15	-5.918	-6.156	-5.000e-06	0.00714	0.46	0.654
sns_001_01616	In ₄ Yb ₈	12	-2.381	-2.109	4.000e-06	0.00288	0.106	0.075
sns_001_01617	Gd ₈ Ge ₆ Pd	15	-5.125	-5.327	-2.100e-05	0.00725	0.494	1.179
sns_001_01642	Al ₁₀ Nd ₅	15	-4.153	-4.273	-6.000e-06	0.00433	0.387	0.947
sns_001_01645	La ₂ Mn ₄ Sn ₅	11	-5.406	-5.966	-2.000e-06	0.00623	0.687	1.737
sns_001_01658	Ga ₆ RhTb ₇	14	-4.395	-4.499	-2.000e-06	0.00296	0.219	0.371
sns_001_01704	Al ₃ Yb ₇ Zn ₃	13	-1.862	-2.056	0.000e+00	0.00418	1.103	1.02
sns_001_01707	Ce ₃ Co ₃ Fe ₄ Sb	11	-6.716	-6.95	-2.400e-05	0.00647	0.429	0.612
sns_001_01718	Gd ₈ Ge ₃ Zn	12	-4.534	-4.609	-1.000e-06	0.00427	0.305	0.255
sns_001_01726	Co ₅ MgNiSi ₄	11	-5.901	-6.109	-2.100e-05	0.00614	0.665	1.023
sns_001_01741	AlGaNd ₅ RhRuSi ₆	15	-5.618	-5.762	0.000e+00	0.00226	0.308	1.012
sns_001_01748	Ce ₂ CoDy ₄ Si ₈	15	-5.491	-5.72	-1.000e-05	0.00737	0.631	1.326
sns_001_01770	Al ₉ Gd ₄ Pb ₂ Sc	16	-4.2	-4.324	-1.000e-06	0.00293	0.475	0.57
sns_001_01771	Ca ₄ Ga ₃ Gd ₄	11	-3.223	-3.314	-1.000e-06	0.00437	0.452	0.357
sns_001_01778	Ge ₅ Tb ₄ Yb ₆	15	-3.863	-3.904	-1.000e-06	0.00338	0.169	0.18
sns_001_01779	AlCo ₁₂ FeGaMn	16	-6.608	-6.735	0.000e+00	0.00804	0.206	0.326
sns_001_01801	B ₆ Ru ₅ U	12	-7.842	-8.185	0.000e+00	0.00548	0.279	0.455
sns_001_01806	Cd ₅ Pt ₄ Sn ₂ Tb ₄ Th	16	-4.119	-4.268	0.000e+00	0.00521	0.283	0.825
sns_001_01846	Nd ₆ Zn ₉	15	-2.569	-2.767	1.000e-06	0.00369	0.639	0.863
sns_001_01852	AlNd ₉ Ru ₄	14	-5.952	-6.094	2.000e-06	0.00266	0.645	1.327
sns_001_01864	Dy ₅ Hf ₅ Ni ₅	15	-6.666	-6.83	0.000e+00	0.00912	0.834	0.795
sns_001_01879	Al ₁₁ Tb ₅	16	-4.026	-4.279	0.000e+00	0.00392	0.435	0.841
sns_001_01892	Ba ₅ Sn ₆ Tb ₄	15	-3.8	-3.881	-6.000e-06	0.00426	0.306	1.476
sns_001_01893	Nd ₈ Ni ₄ Sn ₄	16	-5.1	-5.151	-8.000e-06	0.00585	0.586	0.63
sns_001_01928	Ir ₂ Sn ₅ Yb ₅	12	-3.977	-4.158	1.000e-06	0.00623	0.557	1.286
sns_001_01931	Gd ₆ I ₂ Ru ₂	10	-4.797	-5.268	-1.100e-05	0.00603	0.64	1.214
sns_001_01951	Al ₂ Ge ₆ HfRu ₅ Tc	15	-6.657	-6.861	0.000e+00	0.00885	0.319	0.782
sns_001_01959	Ru ₂ Si ₇ Tb ₆	15	-5.909	-6.134	0.000e+00	0.00444	0.804	2.379
sns_001_01976	Co ₄ Ge ₄ Tb ₈	16	-5.384	-5.568	1.000e-06	0.00767	0.353	0.503
sns_001_01994	As ₃ IrMn ₂ Si ₄ Tb ₆	16	-5.803	-6.23	-1.200e-05	0.00755	1.56	3.025
sns_001_02052	Pt ₅ Yb ₁₀	15	-3.896	-3.939	0.000e+00	0.00306	0.27	0.202
sns_001_02072	Ge ₂ Ni ₄ Si ₄ Tb ₆	16	-5.389	-5.494	-1.000e-06	0.00824	0.277	0.82

Table S9. The profile of generated materials with Snub square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sns_001_02101	Al ₆ Dy ₆ Ga ₂	14	-4.003	-4.302	-1.000e-06	0.00322	0.76	1.558
sns_001_02118	Ge ₅ Nd ₁₀	15	-4.952	-5.215	2.000e-06	0.00451	0.608	0.49
sns_001_02128	GeISb ₂ Tb ₄ Te ₅	13	-4.176	-4.548	-4.000e-06	0.00304	1.058	3.368
sns_001_02138	C ₃ Al ₂ LaRu ₅	11	-7.209	-7.74	2.000e-06	0.00977	0.839	0.729
sns_001_02143	Al ₄ PrSmTb ₈	14	-4.45	-4.479	-3.000e-06	0.00513	0.138	0.708
sns_001_02146	Fe ₅ Tb ₈	13	-5.691	-5.834	-1.000e-06	0.00448	0.63	1.416
sns_001_02147	AlCdCoGaGd ₇ Si ₄ Zn	16	-4.562	-4.735	-3.000e-06	0.00824	0.713	1.657
sns_001_02157	Ce ₂ Ga ₇ Nd ₄ Sn	14	-3.993	-4.427	-2.000e-06	0.0042	1.048	3.318
sns_001_02161	Ge ₇ Ru ₄ SnTi	13	-5.679	-6.156	0.000e+00	0.0079	0.584	0.791
sns_001_02174	Ga ₄ Nd ₈ Ni ₄	16	-4.663	-4.794	2.000e-06	0.00469	0.73	1.985
sns_001_02180	Ga ₈ Gd ₈	16	-4.153	-4.333	0.000e+00	0.00388	0.349	0.471
sns_001_02199	EuGd ₅ Ir ₃ Tl ₂	11	-5.259	-5.616	-5.000e-06	0.00662	1.322	2.833
sns_001_02208	CaPd ₆ Tb ₇	14	-5.174	-5.327	0.000e+00	0.00985	0.51	0.675
sns_001_02260	Gd ₈ Ru ₅	13	-6.299	-6.62	0.000e+00	0.00616	0.731	1.623
sns_001_02265	Cd ₃ Ga ₂ Gd ₅ SbTl ₅	16	-2.968	-3.167	1.000e-06	0.00833	0.574	0.611
sns_001_02270	CdIrNd ₇ OsPt	11	-5.697	-5.776	-1.400e-05	0.00647	0.395	0.313
sns_001_02306	Dy ₇ Ga ₂ GePd ₄	14	-4.994	-5.08	-5.000e-06	0.00516	0.438	1.416
sns_001_02310	Ga ₂ OsRu ₁₀ SmTa	15	-7.745	-8.207	0.000e+00	0.0086	0.3	0.741
sns_001_02315	Al ₉ La ₃ Tb ₄	16	-4.157	-4.442	1.000e-06	0.00453	0.756	1.923
sns_001_02357	B ₅ GeRu ₈	14	-7.765	-7.942	0.000e+00	0.00496	0.302	0.774
sns_001_02364	Gd ₇ GeIrPd ₂ RuSn	13	-5.714	-5.871	-2.000e-06	0.00669	0.349	1.531
sns_001_02383	Ge ₃ Mn ₅	8	-6.891	-7.119	-2.000e-05	0.00423	0.53	0.525
sns_001_02416	Dy ₅ Ga ₅ Rh ₄	14	-4.956	-5.382	1.000e-06	0.00853	0.965	1.735
sns_001_02421	Sn ₅ Sr ₄ Tb ₇	16	-3.814	-3.98	-3.000e-06	0.00278	0.657	1.512
sns_001_02433	Mn ₉ Ni ₆ Si	16	-7.224	-7.443	0.000e+00	0.00879	0.256	1.393
sns_001_02436	Co ₃ Ho ₈ Tb ₄	15	-4.988	-5.126	-9.000e-06	0.00937	0.705	1.677
sns_001_02447	Fe ₅ Gd ₂ Ni ₂ Zn	10	-5.759	-6.099	8.000e-06	0.00651	0.792	0.672
sns_001_02455	AlCo ₂ Gd ₇	10	-4.888	-5.111	1.000e-06	0.0075	0.873	0.903
sns_001_02457	CaGe ₂ Ni ₇	10	-4.907	-5.094	-1.000e-06	0.00464	0.322	0.962
sns_001_02471	Fe ₄ GaMn ₉ SiTi	16	-7.937	-8.14	-2.000e-05	0.00546	0.749	1.341
sns_001_02479	Ir ₄ Se ₂ Sn ₆ Tb ₄	16	-5.559	-5.729	0.000e+00	0.005	0.342	1.016
sns_001_02491	Tb ₆ Tl ₉	15	-3.276	-3.365	0.000e+00	0.00448	0.792	0.834
sns_001_02559	Dy ₄ Ga ₈ Li ₃ Mg	16	-3.209	-3.507	0.000e+00	0.00542	0.965	1.334
sns_001_02579	Ge ₇ Nd ₆ U ₂	15	-4.781	-4.947	1.200e-05	0.00718	0.355	0.993
sns_001_02584	Ga ₉ MgYb ₆	16	-2.477	-2.659	-1.000e-06	0.00479	0.461	0.76
sns_001_02587	Ga ₈ Nd ₆	14	-3.917	-4.151	-2.900e-05	0.00777	0.406	1.222
sns_001_02592	Ag ₄ Al ₃ Nd ₈ Re	16	-4.548	-4.659	3.000e-06	0.00592	0.64	0.733
sns_001_02597	CdS ₈ Tb ₄ Ti	14	-5.361	-5.914	0.000e+00	0.00574	0.727	0.91
sns_001_02621	CdGdGeNd ₉ PtSb	14	-4.871	-4.898	1.000e-06	0.00462	0.282	0.359
sns_001_02628	Al ₇ LiRu ₄	12	-5.348	-5.995	-1.000e-06	0.0077	1.272	2.749
sns_001_02673	Fe ₄ Te ₄	8	-5.183	-5.667	9.000e-06	0.00635	0.835	1.0
sns_001_02675	Al ₅ HfRu ₅ Si ₄	15	-6.585	-6.749	0.000e+00	0.00631	0.448	1.719
sns_001_02678	AlGd ₅ Ge ₇ Ti ₂ U	16	-5.523	-5.757	-2.000e-06	0.00504	0.528	1.559
sns_001_02691	CoGa ₉ Nd ₆	16	-4.079	-4.283	-3.000e-06	0.00422	1.261	1.885
sns_001_02710	AlDy ₆ Ga ₂ Pr ₂ Rh ₂	13	-4.917	-5.082	1.000e-06	0.00569	0.762	1.534
sns_001_02732	CoCrFe ₉ MoSi ₃ V	16	-7.835	-8.048	-1.000e-05	0.00548	1.058	1.373
sns_001_02738	LaPt ₇ SnYb ₆	15	-4.743	-4.937	0.000e+00	0.00695	0.565	0.935
sns_001_02748	Ge ₃ Nd ₆ Pt ₄	13	-5.577	-5.844	-4.000e-06	0.00623	0.601	1.225
sns_001_02772	GeMgRuTb ₇	10	-4.842	-4.961	-1.000e-06	0.00352	0.695	0.531
sns_001_02780	LiNa ₄ Ni ₅ S ₅	15	-4.02	-4.178	-1.800e-05	0.00926	0.835	1.495
sns_001_02793	GePd ₆ Tb ₈	15	-5.331	-5.513	-2.000e-06	0.00401	0.479	1.998
sns_001_02795	Ga ₆ NbRu ₈ Ti	16	-6.913	-7.229	0.000e+00	0.00364	0.874	2.006

Table S9. The profile of generated materials with Snub square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sns_001_02809	Ca ₂ Fe ₅ P ₆	13	-6.121	-6.487	0.000e+00	0.00516	0.364	1.782
sns_001_02845	Al ₁₁ Fe ₄	15	-4.844	-5.132	-7.000e-06	0.0084	1.1	2.128
sns_001_02867	Ga ₇ Tb ₅ YYb ₂	15	-3.74	-4.023	-7.000e-06	0.00372	0.929	1.195
sns_001_02874	Ga ₃ Gd ₈ Tl ₂	13	-3.979	-4.152	-1.000e-06	0.00625	0.355	2.795
sns_001_02881	Ga ₂ GdNdSn ₄ Yb ₈	16	-3.006	-3.13	-3.000e-06	0.00632	0.774	1.636
sns_001_02894	DyFe ₆ Si ₄	11	-6.875	-7.083	3.000e-06	0.00556	0.416	0.977
sns_001_02928	Dy ₄ Sn ₂	6	-4.527	-4.792	1.000e-06	0.00689	0.944	0.942
sns_001_02959	Ga ₈ Yb ₇	15	-2.485	-2.707	-1.000e-06	0.00257	0.599	1.036
sns_001_02974	GeLi ₆ Mn ₄ Ni ₂ STi	15	-4.704	-5.031	5.380e-04	0.00601	0.706	1.451
sns_001_03002	Gd ₆ Si ₂ Sn ₃	11	-4.637	-5.069	-4.000e-06	0.00319	1.355	3.62
sns_001_03025	CdSb ₃ Yb ₁₀	14	-2.457	-2.468	0.000e+00	0.00304	0.123	0.191
sns_001_03029	Ge ₂ Pd ₂ Ru ₄	8	-6.793	-7.088	-2.000e-06	0.00636	0.189	0.292
sns_001_03032	AlDy ₄ Si ₁₀ V	16	-5.063	-5.622	-4.700e-05	0.00423	0.877	1.596
sns_001_03050	DySn ₂ Tb ₅	8	-4.538	-4.752	-5.000e-06	0.00331	0.807	0.996
sns_001_03055	Sn ₆ Yb ₇	13	-2.849	-3.093	-5.000e-06	0.00281	1.069	1.664
sns_001_03056	Rb ₂ Tl ₂ Yb ₄	8	-1.434	-1.524	-4.000e-06	0.00266	0.849	0.778
sns_001_03059	BiNa ₇ Rh ₂ Yb ₄	14	-2.4	-2.53	-2.000e-06	0.00355	0.667	2.824
sns_001_03091	Au ₂ Dy ₄ Ga ₈ GeNi	16	-3.953	-4.033	-1.000e-06	0.00507	0.157	0.691
sns_001_03095	AgAs ₂ Gd ₅ Ge ₂ Rh ₂ Sn ₂	14	-4.992	-5.254	-1.000e-06	0.00536	0.173	0.936
sns_001_03101	GdRhRu ₅ Sn ₇ Tm	15	-5.807	-6.092	0.000e+00	0.00548	0.738	2.115
sns_001_03117	Gd ₇ Ge ₇ Mn	15	-5.079	-5.383	0.000e+00	0.00288	0.623	2.167
sns_001_03118	AlAu ₂ Ge ₄ Ru ₄ Tb ₅	16	-5.784	-5.955	-1.000e-06	0.00697	0.69	1.032
sns_001_03142	Co ₅ Ga ₅ Gd ₆	16	-4.95	-5.124	-8.100e-05	0.00665	0.415	0.934
sns_001_03145	K ₂ SbSnTb ₄	8	-3.289	-3.628	0.000e+00	0.00436	0.944	0.757
sns_001_03150	Ga ₈ Yb ₈	16	-2.551	-2.721	-1.000e-06	0.00439	0.293	0.873
sns_001_03152	AlGa ₃ LaNd ₈ SnSr ₂	16	-4.047	-4.145	-2.900e-05	0.00569	0.212	1.833
sns_001_03154	Ni ₁₀ Tb ₆	16	-5.228	-5.429	1.200e-05	0.00918	0.378	0.629
sns_001_03164	Ge ₃ Nd ₇ PdPt ₃	14	-5.514	-5.766	-1.000e-06	0.0033	0.407	1.215
sns_001_03167	AgCdCeGa ₆ Tb ₅	14	-3.673	-3.872	-1.000e-06	0.00617	0.904	2.252
sns_001_03168	Pd ₄ Yb ₁₂	16	-2.711	-2.846	-1.100e-05	0.00262	0.573	0.706
sns_001_03170	Mn ₈ Ni ₇ Si	16	-7.078	-7.218	-1.500e-04	0.0072	0.326	0.425
sns_001_03176	Pt ₉ Tb ₆	15	-6.276	-6.485	-1.000e-06	0.00603	0.452	0.972
sns_001_03190	Ga ₆ Nd ₆	12	-4.049	-4.223	-1.000e-06	0.00806	0.731	1.998
sns_001_03198	GaNd ₇ Si ₅ Zn ₂	15	-4.565	-4.752	-8.000e-06	0.00395	0.58	1.096
sns_001_03202	Gd ₅ Lu ₂ Sn	8	-4.285	-4.627	1.000e-06	0.00466	0.48	3.178
sns_001_03208	GeNd ₈ NiSi ₄	14	-5.053	-5.396	1.000e-06	0.00622	0.637	0.937
sns_001_03231	Dy ₄ ErSnTl	7	-3.874	-4.392	-2.000e-06	0.00687	0.79	1.703
sns_001_03247	Dy ₆ Sn ₇	13	-4.284	-4.574	-4.000e-06	0.00641	0.613	0.482
sns_001_03248	Ni ₈ P ₄	12	-5.464	-5.737	6.000e-06	0.00904	0.279	0.975
sns_001_03279	AlNd ₈ Si ₆	15	-5.152	-5.526	-1.000e-06	0.00272	0.52	2.574
sns_001_03296	GdLaSe ₈ Yb ₆	16	-4.541	-4.621	-1.000e-06	0.00385	0.31	0.483
sns_001_03327	Eu ₂ Ni ₂ Sn ₅ Tb ₅	14	-4.461	-4.554	0.000e+00	0.00415	0.448	0.508
sns_001_03331	Ga ₁₀ Tb ₅ Ti	16	-3.904	-4.22	-2.000e-05	0.00511	0.907	2.046
sns_001_03347	Al ₉ Nd ₆	15	-4.279	-4.421	0.000e+00	0.00182	1.11	1.734
sns_001_03364	Cd ₂ GaGe ₄ Yb ₅	12	-2.658	-2.858	-1.000e-06	0.00679	0.651	1.662
sns_001_03377	Al ₇ Dy ₅ ErIrMg	15	-4.443	-4.594	4.000e-06	0.00644	0.446	1.907
sns_001_03396	BiBrDy ₂ RuTb ₄ Te ₃	12	-4.695	-5.012	-5.000e-06	0.00543	0.903	2.703
sns_001_03415	GeIrNd ₈ PtRu	12	-5.777	-5.989	1.000e-06	0.00505	0.549	0.769
sns_001_03450	CuGa ₃ MgNd ₆ Pd ₃	14	-4.451	-4.587	-2.000e-06	0.00354	1.02	1.053
sns_001_03452	AuGe ₄ Nd ₈	13	-4.928	-5.141	-7.000e-06	0.00413	0.094	1.505
sns_001_03466	AgDy ₄ Ga ₇ Pd ₃	15	-4.096	-4.33	0.000e+00	0.00904	0.61	0.902
sns_001_03477	Ga ₈ Gd ₈	16	-4.118	-4.332	4.000e-06	0.00776	0.272	0.351

Table S9. The profile of generated materials with Snub square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sns_001_03496	BaCo ₄ Ge ₃ P ₃	11	-5.304	-5.71	-1.000e-06	0.00907	0.573	2.697
sns_001_03497	Al ₇ Gd ₉	16	-4.274	-4.488	-1.600e-05	0.00433	1.057	1.932
sns_001_03507	Ca ₂ Sn ₆ Yb ₄	12	-2.95	-3.177	-1.000e-06	0.00334	0.618	0.827
sns_001_03515	Au ₂ CaCu ₃ Gd ₄ Na	11	-3.517	-3.792	-4.500e-05	0.00941	1.457	1.153
sns_001_03523	Bi ₆ Rb ₃ Yb ₄	13	-2.841	-2.936	-1.100e-05	0.00387	0.352	1.104
sns_001_03532	FeGd ₆ Si ₉	16	-5.486	-5.697	1.000e-06	0.00744	0.564	1.874
sns_001_03540	Co ₆ Ga ₂ MnSnTi ₂ V	13	-6.311	-6.63	-3.000e-06	0.00814	0.672	0.828
sns_001_03547	Ni ₆ Sn ₂	8	-4.91	-5.247	0.000e+00	0.00773	0.459	0.703
sns_001_03608	Pd ₅ TlYb ₈	14	-3.421	-3.545	-5.000e-06	0.00254	0.38	1.516
sns_001_03628	Nd ₂ Ni ₄	6	-5.11	-5.496	-1.500e-05	0.00986	0.837	1.147
sns_001_03632	Hg ₈ Rb ₄ Tb ₄	16	-1.51	-1.638	-8.000e-06	0.0038	0.972	1.618
sns_001_03639	Ce ₄ Ge ₅ Ru ₅	14	-6.583	-7.042	-3.000e-06	0.00482	0.636	1.609
sns_001_03652	Cu ₂ Ni ₅ Tb ₈	15	-4.909	-5.003	-8.000e-06	0.00936	0.502	1.064
sns_001_03677	Cd ₁₁ Dy ₄	15	-1.774	-1.957	-2.000e-06	0.00421	0.574	1.265
sns_001_03681	Al ₃ Ge ₃ OsPd ₂ Tb ₆	15	-5.186	-5.421	-6.000e-06	0.00474	1.102	1.005
sns_001_03683	Cd ₅ Dy ₆ Mg	12	-2.635	-2.694	-7.000e-06	0.00693	0.383	0.423
sns_001_03689	Ga ₂ RbSn ₃ Yb ₆	12	-2.448	-2.633	1.000e-06	0.00512	0.441	2.505
sns_001_03690	Ga ₆ Gd ₆ La ₄	16	-4.251	-4.385	0.000e+00	0.00332	0.7	1.407
sns_001_03697	CdGa ₈ KNd ₄	14	-3.181	-3.364	-5.000e-06	0.00468	0.796	1.977
sns_001_03698	Ga ₈ Tb ₈	16	-3.868	-4.173	-1.000e-06	0.00561	0.815	1.218
sns_001_03702	Al ₂ Gd ₈ Os ₃ Rh ₂	15	-6.083	-6.486	2.000e-06	0.00495	0.871	1.887
sns_001_03705	Ga ₇ Gd ₇	14	-3.983	-4.233	-1.600e-05	0.00638	0.712	2.273
sns_001_03721	Co ₄ Na ₂	6	-4.001	-4.582	5.000e-06	0.00924	0.857	1.042
sns_001_03744	Gd ₆ Se ₉	15	-5.172	-5.721	-1.000e-06	0.00344	0.976	1.227
sns_001_03761	Gd ₄ Sb ₂ SnSr	8	-3.971	-4.555	2.000e-06	0.00524	2.274	2.113
sns_001_03765	Al ₄ CdDy ₄ GaIrLaRh	13	-4.635	-4.948	-3.000e-06	0.00459	0.888	1.846
sns_001_03820	Al ₈ Mn ₇	15	-6.053	-6.304	-2.000e-06	0.00374	0.797	2.851
sns_001_03846	Ge ₅ La ₂ Tb ₆ Zn	14	-4.714	-4.942	0.000e+00	0.0074	0.371	1.702
sns_001_03847	AlCePd ₃ Ru ₅ Sn ₄ Y	15	-6.062	-6.417	1.000e-06	0.00642	0.793	1.578
sns_001_03874	Ga ₇ Nd ₆	13	-3.968	-4.145	-1.000e-06	0.0099	0.469	1.231
sns_001_03914	Co ₅ GeSn ₂ Tb ₅	13	-5.396	-5.595	-2.500e-05	0.0089	0.829	1.39
sns_001_03927	Fe ₂ PdTb ₁₁	14	-5.001	-5.168	-8.000e-06	0.00432	0.809	1.017
sns_001_03949	Ce ₂ Ge ₉ Ru ₄	15	-5.872	-6.208	-6.000e-06	0.00753	0.888	1.907
sns_001_03962	CoFeGa ₅ Nd ₉	16	-4.639	-4.797	0.000e+00	0.00407	0.701	1.072
sns_001_03973	Dy ₈ Pt ₆	14	-6.062	-6.264	-1.000e-06	0.00494	0.09	0.317
sns_001_03976	EuNaSmTb ₄ Tl	8	-3.28	-3.511	-4.000e-06	0.00426	0.524	1.705
sns_001_03994	Gd ₅ Pd ₉	14	-5.552	-5.731	-4.000e-06	0.00485	0.4	0.562
sns_001_04020	Au ₃ Tb ₁₁	14	-4.456	-4.603	0.000e+00	0.00296	1.013	1.336
sns_001_04022	Dy ₅ Ga ₂ Pd ₉	16	-5.281	-5.475	-1.000e-06	0.00516	0.499	0.932
sns_001_04025	GeNd ₅ RhSi ₉	16	-5.476	-5.771	2.000e-06	0.0044	0.836	1.013
sns_001_04040	Ga ₆ Gd ₇	13	-4.1	-4.267	-5.000e-06	0.00413	0.216	1.74
sns_001_04043	CdSbTb ₅ Tl	8	-3.621	-4.14	1.000e-06	0.00382	1.494	1.727
sns_001_04059	Al ₉ Fe ₇	16	-5.652	-5.772	2.000e-06	0.00642	0.313	0.718
sns_001_04066	CdGa ₇ Gd ₈	16	-3.831	-4.081	1.000e-06	0.00855	0.603	0.93
sns_001_04094	Dy ₄ Mn ₂ Ti ₂ Zn ₇	15	-3.696	-4.015	-4.000e-06	0.00396	1.055	2.764
sns_001_04096	Dy ₈ Ga ₆ Sb	15	-4.129	-4.399	-1.500e-05	0.00552	0.923	1.482
sns_001_04126	P ₆ Ru ₉	15	-7.502	-7.949	0.000e+00	0.00836	0.942	0.865
sns_001_04136	Ga ₂ Pt ₉ Ru ₄	15	-6.143	-6.59	-3.000e-06	0.00637	0.444	1.054
sns_001_04146	Gd ₉ InOs ₅ Sb	16	-6.705	-6.666	-1.000e-05	0.00673	0.713	1.441
sns_001_04159	Ge ₇ Ho ₂ Tb ₇	16	-4.825	-5.123	0.000e+00	0.0081	0.496	0.694
sns_001_04168	Al ₂ CaGaHgNd ₈ Sr	14	-3.876	-3.892	-2.000e-06	0.00357	0.119	0.21
sns_001_04178	Ge ₁₀ Tb ₅	15	-4.537	-5.068	-1.000e-06	0.00558	1.262	2.245

Table S9. The profile of generated materials with Snub square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sns_001_04197	Ge ₃ Ru ₂ Tb ₆	11	-5.529	-5.816	1.000e-06	0.0071	0.708	0.895
sns_001_04221	Co ₆ Ge ₂	8	-6.204	-6.425	3.000e-06	0.00581	0.214	0.364
sns_001_04233	Ce ₂ Ga ₇ Tb ₅	14	-4.174	-4.275	7.000e-06	0.00407	0.606	1.281
sns_001_04241	Ce ₄ Dy ₄ Sc ₂ Si ₆	16	-5.591	-5.797	1.000e-06	0.00942	0.684	1.058
sns_001_04242	Ge ₃ IrNd ₈ OsRh	14	-5.98	-6.075	-5.000e-06	0.0063	0.481	0.556
sns_001_04244	La ₂ Ni ₄	6	-5.257	-5.484	1.000e-06	0.00661	0.913	1.051
sns_001_04245	Ga ₈ MgNd ₆	15	-3.658	-3.998	1.000e-06	0.00438	1.773	1.968
sns_001_04249	Ga ₄ Ir ₃ Nd ₇ Sn ₂	16	-5.302	-5.463	-6.000e-06	0.00476	0.311	0.41
sns_001_04257	Ga ₆ NbRhRu ₄	12	-5.985	-6.172	1.000e-06	0.00281	0.428	0.941
sns_001_04276	AlCr ₃ Ga ₅ Gd ₂ MgTb ₄	16	-4.659	-4.889	0.000e+00	0.00233	0.761	0.814
sns_001_04293	Mg ₆ Nd ₄ Ru ₄ Sn ₂	16	-4.395	-4.7	-3.000e-06	0.00502	0.754	1.223
sns_001_04316	AlRhRu ₆ Si ₆ Ti ₂	16	-7.35	-7.592	0.000e+00	0.00509	0.234	1.206
sns_001_04335	Dy ₆ Ga ₇	13	-3.823	-4.052	-2.000e-06	0.00925	0.584	2.128
sns_001_04344	Ge ₆ Nd ₉	15	-4.918	-5.113	-4.000e-06	0.00389	0.708	1.737
sns_001_04370	Li ₃ Mn ₅ O ₈	16	-6.677	-7.037	-1.086e-01	0.00865	0.685	0.816
sns_001_04379	EuGd ₄ Sn ₆ Sr ₃	14	-3.792	-3.855	0.000e+00	0.00614	0.629	0.543
sns_001_04394	Dy ₇ GaGe ₃ Ir ₃ Pd	15	-5.927	-6.061	-7.000e-06	0.00632	0.304	0.464
sns_001_04419	Gd ₅ GeLiSi ₉	16	-4.948	-5.331	-1.000e-06	0.00886	0.75	1.022
sns_001_04431	Cu ₅ Ga ₂ Nd ₈	15	-4.283	-4.344	-1.200e-05	0.00789	0.214	0.263
sns_001_04442	Gd ₇ GeNi ₆	14	-5.144	-5.31	-4.000e-06	0.00524	0.462	1.5
sns_001_04465	CoNd ₈ Pd ₂ Zn ₂	13	-4.668	-4.728	-2.000e-06	0.00553	0.162	0.7
sns_001_04470	Al ₆ Mn ₄ Pd ₆	16	-5.734	-5.947	-1.200e-05	0.00628	0.416	1.367
sns_001_04488	Al ₂ Ce ₆ Gd ₈	16	-4.865	-5.014	-2.600e-05	0.00486	0.731	0.619
sns_001_04493	Ga ₉ Gd ₅ Ti	15	-4.003	-4.227	4.000e-06	0.00511	1.003	2.068
sns_001_04495	Co ₄ Sn ₅ Tb ₇	16	-5.063	-5.327	3.000e-06	0.0092	0.507	0.754
sns_001_04514	CdDy ₇ Ga ₆	14	-3.858	-4.001	-2.400e-05	0.00532	0.254	1.329
sns_001_04516	Co ₇ Sb ₃	10	-5.702	-5.95	-1.500e-05	0.00899	0.463	0.472
sns_001_04526	Gd ₇ RuSi ₅	13	-5.392	-5.695	1.000e-06	0.00426	0.725	1.473
sns_001_04537	Dy ₆ Ga ₄ Li ₃	13	-3.549	-3.664	0.000e+00	0.00591	0.524	0.698
sns_001_04562	SbSn ₃ Tb ₄	8	-4.137	-4.915	-4.000e-06	0.00514	1.005	1.385
sns_001_04601	Dy ₉ Ga ₇	16	-4.142	-4.246	-6.000e-06	0.00375	0.453	0.931
sns_001_04604	Al ₅ Gd ₈ Ge	14	-4.37	-4.656	-3.000e-06	0.00345	0.756	1.649
sns_001_04609	Ge ₇ Tb ₈	15	-4.968	-5.315	0.000e+00	0.00242	0.707	0.816
sns_001_04614	Ba ₂ CdGe ₃ Sn ₄ Yb ₅	15	-2.953	-3.192	-3.000e-06	0.00388	1.066	3.401
sns_001_04644	Nd ₄ Pb ₂	6	-4.421	-4.696	-1.400e-05	0.00565	0.958	0.813
sns_001_04655	Rh ₄ Sn ₆ Yb ₆	16	-4.123	-4.338	0.000e+00	0.00462	0.842	1.69
sns_001_04664	Rh ₃ SnTb ₇	11	-5.484	-5.786	-6.000e-06	0.00371	0.832	1.516
sns_001_04670	Co ₂ Ge ₄ SmTb ₇ Zn ₂	16	-4.741	-4.865	-2.000e-06	0.00688	0.9	0.764
sns_001_04680	Al ₄ Cu ₂ LiRu ₅	12	-5.777	-6.004	-1.100e-05	0.00753	0.47	0.514
sns_001_04687	Al ₃ GeSn ₄ Tb ₇	15	-4.57	-4.684	0.000e+00	0.00685	0.593	0.705
sns_001_04708	Gd ₆ La ₂ PdPt ₃	12	-5.621	-5.803	-3.000e-06	0.00558	0.691	0.716
sns_001_04717	FeGa ₇ Nd ₇	15	-4.23	-4.409	1.000e-06	0.00614	0.774	1.668
sns_001_04735	Ga ₂ Ni ₂ Si ₅ Tb ₆	15	-5.05	-5.186	-4.000e-06	0.00553	0.341	0.931
sns_001_04736	Co ₅ GaSi ₂ Tb ₈	16	-5.269	-5.62	1.000e-06	0.00699	1.244	1.814
sns_001_04749	ErNi ₉ Ru ₅	15	-6.458	-6.636	1.000e-06	0.00871	0.569	0.817
sns_001_04754	Nd ₈ Ru ₂ Si ₆	16	-5.95	-6.094	-1.000e-06	0.00228	0.695	0.496
sns_001_04762	Ge ₄ NiRu ₄ Sr ₃	12	-5.309	-5.617	-1.000e-06	0.00677	0.249	0.599
sns_001_04767	Ga ₈ Tb ₇	15	-3.886	-4.15	-1.000e-06	0.00677	0.3	1.222
sns_001_04778	Gd ₅ PrSb ₂	8	-4.69	-5.01	3.000e-06	0.00476	0.785	0.806
sns_001_04825	Cd ₄ Dy ₄ Rh ₃ SbTb ₂	14	-4.362	-4.504	-1.000e-06	0.00635	0.27	1.673
sns_001_04830	CoGe ₇ Nd ₅ PtRu	15	-5.372	-5.634	-1.000e-06	0.00903	0.47	1.183
sns_001_04832	Br ₂ K ₂ O ₆ PdTb ₄	15	-5.89	-6.324	-2.000e-06	0.00973	0.523	0.935

Table S9. The profile of generated materials with Snub square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sns_001_04835	MgNd ₇ Pd ₃ SbSn	13	-4.882	-4.995	0.000e+00	0.00425	0.342	0.398
sns_001_04867	CeNi ₄ Sn	6	-5.303	-5.654	-9.000e-06	0.00789	1.042	0.929
sns_001_04881	Pd ₃ Tb ₇ Tl	11	-4.755	-4.999	-4.000e-06	0.00406	0.799	1.163
sns_001_04885	Al ₄ Ce ₄ GeSmTb ₄	14	-4.766	-4.922	-2.500e-05	0.00543	0.223	0.386
sns_001_04919	Ga ₇ Nd ₇ Pr	15	-4.203	-4.377	0.000e+00	0.00613	0.54	0.497
sns_001_04938	Gd ₇ Rh ₇	14	-6.352	-6.545	-3.000e-06	0.00467	0.703	2.194
sns_001_04942	Dy ₈ GaSn ₆	15	-4.457	-4.617	-2.000e-06	0.00601	0.362	1.477
sns_001_04953	Al ₇ CeGaGd ₄ Ge ₂ Mn	16	-4.393	-4.688	-1.800e-05	0.00799	0.454	0.519
sns_001_04967	Gd ₈ Ge ₈	16	-5.079	-5.274	-1.000e-06	0.00504	0.874	1.226
sns_001_04994	Al ₇ Mg ₈ Sn ₂ Tb ₆	16	-4.106	-4.22	-1.000e-06	0.0033	0.303	0.336
sns_001_04995	Al ₁₂ Ru ₄	16	-5.178	-5.351	-7.000e-06	0.00631	0.2	1.145
sns_001_04999	BGeRu ₆ Si ₂ Sn	11	-7.103	-7.418	-3.000e-06	0.00624	0.805	1.84
sns_001_05017	Al ₇ Dy ₈	15	-4.255	-4.367	-3.000e-06	0.00454	0.245	0.383
sns_001_05045	Na ₆ Pb ₂ Tb ₄	12	-2.673	-2.762	-2.000e-06	0.00692	0.307	1.202
sns_001_05048	AlCo ₃ Gd ₈ Si ₄	16	-5.508	-5.64	-9.000e-06	0.00868	0.477	0.637
sns_001_05058	Cu ₇ Ga ₂ Nd ₆	15	-4.025	-4.191	-4.000e-06	0.00541	0.607	0.73
sns_001_05071	Co ₃ Ga ₇ Tb ₆	16	-4.402	-4.696	-5.000e-06	0.00579	0.67	1.492
sns_001_05076	Ge ₆ Ir ₃ Tb ₆	15	-5.708	-5.999	1.000e-06	0.00874	0.69	1.283
sns_001_05079	Al ₄ Gd ₆ Ni ₆	16	-4.789	-5.101	-1.100e-04	0.0071	0.832	2.201
sns_001_05113	Cd ₂ NaSn ₃ Yb ₉	15	-2.031	-2.139	0.000e+00	0.00482	0.469	1.723
sns_001_05125	CeGeRh ₄ Sb ₂ Tb ₆	14	-5.799	-6.047	0.000e+00	0.00591	0.554	0.738
sns_001_05134	Al ₅ Ge ₂ SnTb ₈	16	-4.403	-4.752	0.000e+00	0.00439	0.268	1.359
sns_001_05141	Cd ₂ Ga ₃ Ge ₂ RuSiTb ₇	16	-4.503	-4.61	0.000e+00	0.00303	0.367	0.268
sns_001_05156	As ₃ Sb ₂ Si ₃ Tb ₈	16	-5.386	-5.626	0.000e+00	0.00293	0.467	0.578
sns_001_05160	K ₂ Nd ₄	6	-2.719	-3.173	0.000e+00	0.00528	2.552	2.358
sns_001_05206	Ba ₂ Nd ₆ Sn ₇	15	-4.144	-4.353	0.000e+00	0.00339	1.001	3.113
sns_001_05243	Al ₂ CoMn ₆ MoSc ₂ Tc ₄	16	-8.091	-8.334	1.000e-05	0.00599	0.639	0.747
sns_001_05265	CoGa ₇ Tb ₆	14	-4.079	-4.218	-3.000e-06	0.0085	0.554	0.481
sns_001_05271	LaTb ₅ Tl ₂	8	-4.04	-4.216	-4.900e-05	0.00461	0.357	0.539
sns_001_05290	CeNi ₄ Sn ₂ Sr	8	-4.723	-5.036	2.000e-06	0.00715	0.795	0.848
sns_001_05294	Ga ₅ Nd ₈	13	-4.206	-4.397	-3.000e-06	0.00569	0.854	2.06
sns_001_05301	Ga ₉ Gd ₅	14	-3.547	-3.904	-1.000e-06	0.00934	0.382	0.594
sns_001_05332	Dy ₄ Ga ₄ Pd ₆	14	-4.914	-5.105	1.000e-06	0.0091	0.668	1.445
sns_001_05334	Pd ₉ Tb ₆	15	-5.543	-5.725	0.000e+00	0.00537	0.708	1.619
sns_001_05335	Dy ₈ Pt ₄	12	-5.887	-5.916	0.000e+00	0.0055	0.177	0.193
sns_001_05346	Co ₃ Sn ₄ Tb ₄	11	-4.886	-5.265	0.000e+00	0.00842	1.091	2.09
sns_001_05350	Ga ₉ Yb ₇	16	-2.523	-2.802	-5.000e-06	0.00574	1.174	1.854
sns_001_05398	Pd ₃ Sn ₂ Yb ₆	11	-3.281	-3.608	-5.000e-06	0.0048	1.533	2.501
sns_001_05413	AlGaMn ₄ Ni ₆	12	-6.115	-6.396	-6.000e-06	0.00942	0.532	0.634
sns_001_05429	Ni ₄ SnTb	6	-5.097	-5.388	4.000e-06	0.00638	0.427	1.501
sns_001_05443	AgGeLiNi ₅	8	-4.373	-4.62	0.000e+00	0.00763	0.602	0.529
sns_001_05447	Co ₃ GeSbSnTb ₈	14	-5.118	-5.368	-2.600e-05	0.00382	1.153	2.177
sns_001_05456	Ga ₄ SbTb ₇	12	-4.275	-4.418	-2.000e-06	0.00672	0.61	2.206
sns_001_05478	CCo ₂ Fe ₄ Ga ₃ Ni ₃	13	-6.091	-6.263	1.000e-06	0.0059	0.346	0.451
sns_001_05481	CuGa ₂ Gd ₈ Y ₂	13	-4.493	-4.673	6.000e-06	0.00404	0.958	1.361
sns_001_05495	CoGa ₅ IrLiNd ₈	16	-4.497	-4.729	-7.000e-06	0.00759	0.398	2.03
sns_001_05511	Al ₁₀ Gd ₆	16	-4.221	-4.353	-2.000e-06	0.00329	0.566	1.407
sns_001_05534	Ga ₄ Nd ₆ Sn ₃	13	-4.144	-4.413	-1.000e-06	0.00531	0.526	1.707
sns_001_05598	Dy ₇ La ₅ Tc ₂	14	-5.414	-5.451	-2.000e-06	0.00691	0.171	1.152
sns_001_05602	Ga ₄ Gd ₈	12	-4.131	-4.357	-8.000e-06	0.00352	1.236	1.584
sns_001_05615	Dy ₈ Rh ₄	12	-5.98	-6.001	-3.000e-06	0.0044	0.33	0.31
sns_001_05616	GaGe ₂ Ni ₂ Pd ₂ Ru ₄	11	-6.211	-6.443	-1.000e-06	0.00721	0.843	2.299

Table S9. The profile of generated materials with Snub square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sns_001_05623	Cd ₂ Ce ₂ P ₆ Tb ₆	16	-5.443	-5.48	1.000e-06	0.00416	0.059	1.012
sns_001_05631	As ₂ CaGaMgRu ₄ Tb ₅	14	-5.401	-5.84	1.000e-06	0.00841	1.661	2.672
sns_001_05632	Al ₄ CoGd ₇ Si ₄	16	-4.983	-5.122	-6.000e-06	0.00321	0.234	0.832
sns_001_05666	Ga ₅ Tb ₆ Yb ₂	13	-3.698	-3.807	0.000e+00	0.00225	0.089	0.801
sns_001_05675	Co ₆ Tb ₈	14	-5.484	-5.691	3.000e-06	0.00991	0.722	1.115
sns_001_05702	Co ₈ GdGe ₂ Ni ₂ P	14	-6.094	-6.249	5.000e-06	0.00594	0.233	0.681
sns_001_05729	Nd ₆ PdPt ₇	14	-5.988	-6.234	2.000e-06	0.00652	1.258	1.484
sns_001_05774	AlCaDy ₄ Pr	7	-3.887	-4.001	-1.000e-06	0.00439	0.418	2.241
sns_001_05786	LaTb ₅ Tl ₂	8	-3.925	-4.19	0.000e+00	0.00268	1.412	1.228
sns_001_05803	Gd ₇ Pt ₃ Si	11	-5.525	-5.808	2.000e-06	0.00398	1.019	3.669
sns_001_05819	CoFe ₁₀ Mn ₂ Ni ₂ V	16	-7.702	-7.842	-2.000e-05	0.00529	0.227	0.373
sns_001_05824	Dy ₆ Ga ₁₀	16	-3.693	-3.943	2.000e-06	0.0086	0.717	1.921
sns_001_05830	Gd ₆ Ge ₉ Rh	16	-5.039	-5.286	-6.000e-06	0.0029	0.379	1.058
sns_001_05875	Ni ₅ P ₉ Pr	15	-5.338	-5.664	-6.000e-06	0.00658	0.959	2.458
sns_001_05889	Al ₅ Dy ₆ Fe ₅	16	-5.365	-5.512	4.000e-06	0.00734	0.413	0.982
sns_001_05902	Cd ₂ Gd ₁₀ MgPt ₃	16	-4.436	-4.691	0.000e+00	0.00291	0.36	1.568
sns_001_05908	Ce ₂ Fe ₅ Si ₆ Zn	14	-6.161	-6.629	0.000e+00	0.0055	1.242	2.111
sns_001_05917	AlGe ₄ Mn ₅ SiTa	12	-6.673	-6.945	-2.000e-05	0.00565	0.549	1.576
sns_001_05948	Gd ₄ Tl ₄	8	-3.377	-3.785	-4.000e-06	0.00443	0.858	1.405
sns_001_05967	Al ₇ MnNd ₈	16	-4.636	-4.776	-8.000e-06	0.00602	0.582	1.699
sns_001_06054	Ru ₄ Sn ₄ Zn ₅	13	-4.151	-4.347	-4.000e-06	0.00879	0.57	0.716
sns_001_06061	CaGe ₂ NdPt ₄ Tb ₅ Tl	14	-5.178	-5.463	-3.000e-06	0.00472	0.651	1.27
sns_001_06065	La ₂ Nd ₅ Pd ₇	14	-5.346	-5.616	-5.000e-06	0.0055	0.644	1.011
sns_001_06067	Dy ₈ RhRu	10	-5.301	-5.537	-8.000e-06	0.00285	0.538	0.697
sns_001_06096	GaNi ₁₁ SnYb	14	-4.853	-4.976	-2.700e-05	0.00507	0.358	0.746
sns_001_06111	Pd ₆ RhSnTb ₅	13	-5.519	-5.746	-1.400e-05	0.00731	0.652	0.884
sns_001_06142	P ₂ Ru ₇ Si ₆ W	16	-7.249	-7.818	0.000e+00	0.00762	0.745	1.895
sns_001_06150	Dy ₇ NdRh ₄	12	-5.974	-5.997	-1.200e-05	0.0046	0.424	0.391
sns_001_06155	NbNi ₅ SbSi	8	-5.763	-5.967	-1.000e-06	0.00426	0.431	0.641
sns_001_06156	Pd ₅ Tb ₇	12	-5.307	-5.46	0.000e+00	0.00223	1.114	2.874
sns_001_06174	CoDy ₅ NdPb	8	-4.727	-4.85	-1.300e-05	0.00481	0.098	0.291
sns_001_06199	Dy ₆ MnSi ₈ W	16	-5.787	-6.28	0.000e+00	0.0044	1.037	1.073
sns_001_06201	CdGa ₂ Mn ₃ Tb ₈ Tl	15	-4.701	-4.856	-5.000e-06	0.00556	0.242	0.35
sns_001_06215	Ni ₄ S ₂ Te ₂	8	-4.574	-4.755	-2.700e-05	0.00836	0.525	0.522
sns_001_06232	AgAl ₃ Dy ₅ Pt ₃	12	-5.055	-5.275	-3.000e-06	0.00515	0.765	1.195
sns_001_06236	AlGePd ₄ Yb ₇	13	-3.515	-3.669	-6.000e-06	0.00387	0.827	1.274
sns_001_06252	Ni ₁₁ Sn ₅	16	-4.8	-5.073	-1.800e-05	0.00877	0.916	1.689
sns_001_06273	Co ₆ SiTb ₈	15	-5.558	-5.758	3.000e-06	0.00841	1.081	2.169
sns_001_06282	Au ₄ Mg ₂ Yb ₈	14	-2.548	-2.578	-4.000e-06	0.00547	0.201	0.759
sns_001_06291	FeP ₄ Ru ₇ Ti	13	-8.14	-8.285	0.000e+00	0.00374	0.217	0.196
sns_001_06307	Al ₂ Ga ₆ Gd ₈	16	-4.226	-4.392	7.000e-06	0.00422	0.276	0.381
sns_001_06308	K ₂ Ru ₄ S ₆	12	-5.116	-5.712	-3.000e-06	0.0075	0.597	2.387
sns_001_06315	GeMn ₁₅	16	-8.559	-8.643	-1.000e-05	0.00761	0.142	0.27
sns_001_06325	GaRu ₄ Tb	6	-6.989	-7.391	-7.000e-06	0.00599	0.985	0.915
sns_001_06333	Ga ₈ Yb ₈	16	-2.578	-2.722	2.000e-06	0.00716	0.635	1.251
sns_001_06346	Co ₂ RuSn ₃ Tb ₈	14	-5.085	-5.432	4.000e-06	0.00739	0.795	1.813
sns_001_06374	Ga ₂ Li ₂ RhTb ₇ Zn	13	-3.95	-4.103	-2.000e-06	0.00402	0.558	1.784
sns_001_06380	Al ₇ CuGaRu ₅ Zr	15	-5.942	-6.132	-1.000e-06	0.00992	0.228	0.387
sns_001_06402	As ₄ GeMn ₄ Rb	10	-5.42	-5.982	-1.000e-06	0.00982	0.925	1.659
sns_001_06403	La ₃ Nd ₅ S ₂ Se ₆	16	-5.697	-5.907	3.000e-06	0.00337	0.062	0.318
sns_001_06406	Gd ₉ InSi ₆	16	-5.258	-5.29	2.000e-06	0.0037	0.935	1.835
sns_001_06434	Ge ₆ Pd ₄ Tb ₅ Ti	16	-5.415	-5.569	0.000e+00	0.00894	0.647	1.472

Table S9. The profile of generated materials with Snub square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
sns_001_06438	Gd ₇ Ni ₉	16	-5.101	-5.339	-2.000e-06	0.00672	0.521	0.707
sns_001_06448	AgIr ₂ Pd ₅ Tb ₇	15	-5.768	-5.951	-3.900e-05	0.00415	0.231	0.824
sns_001_06496	LiNd ₈ Sn ₃	12	-4.484	-4.571	1.000e-06	0.00248	0.805	0.558
sns_001_06517	Nd ₈ Pt ₅ Si ₂	15	-5.753	-6.033	0.000e+00	0.00718	0.61	0.572
sns_001_06541	Ga ₈ Yb ₈	16	-2.544	-2.715	-1.260e-04	0.00706	0.439	1.588
sns_001_06599	CoCuGa ₄ Nd ₇	13	-4.486	-4.587	0.000e+00	0.00424	0.629	0.701
sns_001_06623	Al ₇ Dy ₇ Tc	15	-4.544	-4.789	1.000e-06	0.00349	1.086	1.358
sns_001_06632	Ga ₂ GeRu ₁₀ SiVW	16	-8.057	-8.184	0.000e+00	0.00396	0.127	1.171
sns_001_06644	Mn ₅ Ni ₉ V	15	-6.543	-6.737	0.000e+00	0.00655	0.381	1.381
sns_001_06682	Ga ₈ Yb ₈	16	-2.5	-2.719	-3.000e-06	0.00725	0.37	0.459
sns_001_06690	Co ₈ Si ₈	16	-6.364	-6.662	0.000e+00	0.00808	0.31	0.396
sns_001_06691	Co ₇ Dy ₆ Ga ₂	15	-5.3	-5.65	-2.200e-05	0.0088	0.888	1.736
sns_001_06699	NbNdP ₃ Ru ₆ SbW ₂	14	-8.097	-8.555	0.000e+00	0.00899	0.301	0.939
sns_001_06705	Ge ₄ Pd ₃ SbTb ₆	14	-5.212	-5.347	-1.600e-05	0.00595	0.321	1.172
sns_001_06709	LaMn ₄ Sn	6	-6.678	-7.352	-4.000e-06	0.00712	0.797	1.055
sns_001_06717	AlGaGe ₂ Mn ₁₁ Pd	16	-7.201	-7.463	0.000e+00	0.00531	0.368	0.928
sns_001_06749	AgRh ₂ RuTb ₇	11	-5.472	-5.702	0.000e+00	0.00556	0.913	1.544
sns_001_06752	Ga ₅ Ru ₇	12	-6.318	-6.678	-1.000e-06	0.00402	0.756	1.336
sns_001_06781	Ga ₅ Nd ₄ Rb ₃	12	-2.791	-3.07	-3.000e-06	0.00499	0.895	1.77
sns_001_06796	Al ₇ Nd ₈	15	-4.241	-4.565	0.000e+00	0.0037	0.747	2.465
sns_001_06801	CuGa ₄ GeTb ₈	14	-4.104	-4.338	-6.000e-06	0.00842	0.98	1.135

Table S10. The profile of generated materials with Truncated square lattice structures after DFT relaxation

Index	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tsq_000_00029	Co ₆ Sn ₈	14	-4.87	-5.079	1.000e-06	0.00644	0.288	0.807
tsq_000_00103	Na ₄ Ni ₄ Sn ₂	10	-3.149	-3.5	1.000e-06	0.00542	1.484	1.863
tsq_000_00149	Hf ₅ Ru ₄ Si ₆ Ti	16	-8.032	-8.463	-1.000e-05	0.0056	0.637	1.586
tsq_000_00227	Fe ₅ Se ₆ Tl ₂	13	-4.935	-5.229	-1.100e-05	0.00816	0.93	0.899
tsq_000_00322	Er ₃ Fe ₅ Sn ₅	13	-5.511	-5.705	-6.000e-06	0.00737	0.654	0.608
tsq_000_00349	Cs ₉ Nd ₄	13	-1.465	-1.626	6.000e-06	0.00182	1.375	1.06
tsq_000_00396	DyGa ₇ Mn ₅ PrU	15	-5.456	-5.896	1.000e-06	0.00733	0.895	2.0
tsq_000_00427	Al ₆ Ce ₃ Fe ₄	13	-5.529	-5.823	-7.300e-05	0.00857	0.722	0.677
tsq_000_00455	FeNi ₆ Sn ₈	15	-4.456	-4.813	3.000e-06	0.00722	0.684	2.673
tsq_000_00473	AgEuGe ₂ Ni ₇ Sb	12	-4.557	-4.887	-1.300e-05	0.00864	0.931	0.836
tsq_000_00485	CaCe ₄ Ga ₆ Ru ₄	15	-5.203	-5.638	-4.000e-06	0.00461	0.867	1.329
tsq_000_00548	Cs ₅ SnYb ₄	10	-1.147	-1.301	1.000e-06	0.00265	1.397	2.259
tsq_000_00601	Cs ₅ Nd ₄	9	-1.643	-2.177	-1.200e-05	0.00912	3.144	3.228
tsq_000_00646	I ₈ Nd ₄	12	-3.56	-3.819	-5.000e-06	0.00439	0.735	2.2
tsq_000_00647	Ca ₃ Ni ₉ Si	13	-4.568	-4.767	-2.210e-04	0.00871	0.469	0.51
tsq_000_00678	CdGe ₃ Nd ₂ Ni ₄	10	-4.489	-4.93	5.000e-06	0.00893	0.804	1.06
tsq_000_00704	Cs ₅ RbYb ₆	12	-0.788	-0.982	-1.000e-06	0.00356	2.109	1.935
tsq_000_00726	Al ₃ Ni ₄ P ₇ Ti	15	-5.162	-5.514	-7.000e-06	0.00709	1.435	1.409
tsq_000_00757	Co ₅ Ge ₂ Sn ₄ Sr ₅	16	-4.125	-4.301	3.000e-06	0.00524	0.951	1.072
tsq_000_00784	AlGe ₂ Ho ₆ Ru ₄ Si ₃	16	-5.972	-6.321	0.000e+00	0.00749	0.599	0.834
tsq_000_00798	Ru ₅ Sn ₈	13	-5.467	-5.822	9.000e-06	0.00899	0.489	1.844
tsq_000_00866	Cd ₂ Hf ₂ KRu ₄ Zn ₇	16	-3.785	-4.071	5.000e-06	0.00702	0.443	0.454
tsq_000_00868	AgGeNi ₆ Tb ₄	12	-5.01	-5.252	-8.700e-05	0.00731	0.677	0.759
tsq_000_00932	CdCo ₇ Ga ₆ Y ₂	16	-4.963	-5.159	1.000e-06	0.00932	0.86	1.222
tsq_000_00945	EuGe ₂ Sb ₈ SrTb ₄	16	-3.976	-4.541	0.000e+00	0.00815	2.075	2.424
tsq_000_00952	Cs ₅ Yb ₄	9	-0.78	-0.915	-2.100e-06	0.00325	1.585	1.433
tsq_000_01006	GeRu ₆ Sn ₂ UZnZr ₅	16	-7.368	-7.959	0.000e+00	0.00759	0.744	1.687
tsq_000_01015	Br ₃ ClRu ₄	8	-4.322	-5.209	-5.500e-05	0.00989	1.381	2.84
tsq_000_01017	Au ₃ ErMn ₄ Sn ₈	16	-4.587	-4.969	-8.000e-06	0.00913	0.882	1.423
tsq_000_01038	Cs ₅ Tb ₄	9	-1.49	-1.877	-4.000e-06	0.00328	1.467	0.94
tsq_000_01064	Br ₄ Mn ₄	8	-4.478	-5.096	0.000e+00	0.00706	1.155	1.237
tsq_000_01065	AlEr ₂ Ge ₇ Mn ₄	14	-5.506	-5.802	4.000e-06	0.00966	0.782	1.403
tsq_000_01089	Na ₄ Ni ₆ Sn	11	-3.372	-3.53	0.000e+00	0.00727	0.677	0.676
tsq_000_01092	Co ₄ Sn ₆ Sr ₂	12	-4.398	-4.583	-2.300e-05	0.00999	0.781	0.898
tsq_000_01100	Ru ₆ Se ₆	12	-5.768	-6.191	0.000e+00	0.00424	0.905	1.239
tsq_000_01106	Fe ₈ Ge ₆ HoSi	16	-6.173	-6.445	0.000e+00	0.0088	0.652	1.423
tsq_000_01183	Co ₄ Ge ₈ Li ₂ Nd ₂	16	-4.761	-5.049	-3.000e-05	0.00696	0.784	2.326
tsq_000_01195	GeNi ₄ S ₇	12	-4.465	-4.737	-1.000e-06	0.00675	0.41	0.453
tsq_000_01279	I ₄ Ni ₄	8	-3.1	-3.424	-3.000e-06	0.00532	1.141	3.768
tsq_000_01389	Cs ₅ Gd ₄	9	-1.525	-1.899	0.000e+00	0.003	1.414	1.296
tsq_000_01402	Fe ₄ Pt ₉ Tb ₂	15	-6.257	-6.765	-1.000e-05	0.00972	1.791	1.985
tsq_000_01454	CINi ₅ P ₇	13	-4.857	-5.251	-2.000e-06	0.00834	0.901	2.142
tsq_000_01485	CdNd ₄ Sb ₅ SnTe ₃	14	-3.702	-4.469	-1.000e-06	0.00467	2.384	2.354
tsq_000_01520	Mn ₅ Sn ₉	14	-4.783	-5.377	0.000e+00	0.00657	0.914	2.255
tsq_000_01588	Mn ₄ S ₇ Tl	12	-5.609	-5.927	-3.000e-06	0.00593	0.474	0.547
tsq_000_01596	ErMgRu ₆ Sn ₈	16	-5.458	-5.79	-6.000e-06	0.00942	0.707	1.434
tsq_000_01600	Co ₇ Hf ₆ Nb	14	-8.319	-8.717	0.000e+00	0.00957	1.176	1.326
tsq_000_01670	AgGeMn ₄ Sn ₆	12	-4.841	-5.24	-2.800e-05	0.00903	0.848	1.415
tsq_000_01747	Ge ₃ Mn ₄ Pt ₂ Sb ₃	12	-5.703	-6.068	-1.400e-05	0.00688	1.199	1.346
tsq_000_01770	Br ₄ Ru ₄	8	-3.944	-5.058	2.000e-06	0.0098	1.92	2.616
tsq_000_01779	RbRu ₇ Sn ₄ B ₃	15	-5.692	-6.093	1.000e-06	0.00372	0.786	0.785
tsq_000_01785	As ₇ LaMn ₄ TeTi ₂	15	-6.081	-6.545	-1.600e-05	0.00625	0.779	0.737

Table S10. The profile of generated materials with Truncated square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tsq_000_01827	HgMn ₄ NaSe ₅	11	-4.594	-5.028	-2.000e-06	0.00463	1.022	1.461
tsq_000_01949	Ga ₃ Na ₂ Ni ₅ Sr ₃	13	-3.21	-3.457	5.000e-06	0.00942	1.363	1.614
tsq_000_01956	Br ₂ Cs ₃ IRu ₄ Se ₂	12	-4.107	-4.569	-3.400e-05	0.00742	0.84	1.477
tsq_000_01965	Al ₃ Ga ₂ Mn ₅ Pr ₂	12	-5.619	-6.047	-3.000e-06	0.00655	0.547	0.654
tsq_000_01988	Er ₆ GaRu ₇	14	-6.631	-6.935	-1.200e-05	0.00894	0.685	1.484
tsq_000_02031	Co ₄ GeSnSr ₃	9	-4.047	-4.557	-1.700e-05	0.00922	0.776	1.969
tsq_000_02052	Ce ₂ GeMn ₄ NiP ₃ Si ₂	13	-6.494	-6.845	2.000e-06	0.00612	0.647	1.133
tsq_000_02158	Cs ₈ Dy ₄ Li	13	-1.507	-1.633	-9.000e-06	0.00635	1.226	1.041
tsq_000_02219	Co ₃ Mn ₄ NiSn ₇	15	-5.315	-5.741	-2.000e-06	0.00736	0.811	1.34
tsq_000_02223	Dy ₄ I ₈	12	-3.464	-3.571	-3.000e-06	0.0059	0.753	1.423
tsq_000_02231	Al ₅ LaNi ₆ ThY	14	-5.255	-5.406	-1.000e-06	0.00844	0.327	0.861
tsq_000_02236	Lu ₄ Mn ₄ Si ₈	16	-6.008	-6.464	0.000e+00	0.0064	0.993	1.877
tsq_000_02263	Co ₆ Ga ₅ Ho ₃	14	-4.985	-5.239	-1.000e-06	0.00716	0.642	0.579
tsq_000_02277	Al ₉ Fe ₄ Pd	14	-4.919	-5.279	-8.000e-06	0.0033	1.042	1.116
tsq_000_02338	Mn ₄ Ni ₄ Sn ₅	13	-5.239	-5.797	-9.000e-06	0.00847	0.268	1.103
tsq_000_02444	Fe ₄ Ga ₅ GeSn ₃	13	-4.464	-4.762	-7.000e-06	0.00445	0.311	2.005
tsq_000_02451	Ni ₄ Sn ₇	11	-4.036	-4.486	-2.300e-05	0.00855	0.559	1.44
tsq_000_02558	Co ₄ Ge ₆ Hf ₅ Te	16	-6.772	-7.05	0.000e+00	0.00965	1.282	1.274
tsq_000_02598	Ce ₂ Ga ₆ Ni ₆	14	-4.592	-4.836	-7.000e-06	0.00553	1.094	0.886
tsq_000_02602	AgCa ₄ Ge ₂ Ru ₅ Sn ₂	14	-5.073	-5.351	1.000e-06	0.0032	0.855	2.539
tsq_000_02604	Fe ₄ NiSi ₉ Sm ₂	16	-6.0	-6.272	0.000e+00	0.00559	0.432	1.298
tsq_000_02658	BiPrSn ₈ Tb ₄	14	-3.969	-4.672	-2.000e-06	0.00462	1.149	2.524
tsq_000_02677	LiMn ₆ NiSn ₅	13	-5.332	-5.977	-1.000e-05	0.00819	1.284	2.216
tsq_000_02683	Co ₇ GaLi ₄ SbSn ₂	15	-4.425	-4.706	4.651e-03	0.00416	0.796	1.128
tsq_000_02715	Cl ₁₀ Dy ₄ Rb ₂	16	-4.112	-4.276	-6.000e-06	0.00501	1.309	1.531
tsq_000_02727	Al ₅ Ce ₂ Fe ₅	12	-5.674	-6.094	-3.000e-06	0.00533	0.648	0.956
tsq_000_02771	Mn ₅ Pd ₈ Y	14	-6.259	-6.635	-9.800e-05	0.00566	0.674	1.106
tsq_000_02807	Co ₈ Sc ₆	14	-6.561	-6.824	0.000e+00	0.00973	0.872	1.621
tsq_000_02826	Al ₅ Ce ₂ Mn ₅	12	-5.872	-6.377	1.000e-06	0.00735	1.022	0.983
tsq_000_02848	Ni ₁₀ Sn ₆	16	-4.647	-4.917	0.000e+00	0.00872	0.746	1.687
tsq_000_02921	BCo ₄ I ₆	11	-3.427	-3.815	-1.700e-05	0.00728	1.244	2.601
tsq_000_02924	Li ₆ Ni ₈ Si	15	-3.857	-4.146	-5.000e-06	0.00742	0.721	0.801
tsq_000_02954	Co ₄ Ga ₇ MgTb ₂	14	-4.123	-4.519	-1.000e-06	0.00417	0.546	1.078
tsq_000_02958	GeMn ₄ P ₃ Pr ₃ Sb	12	-6.359	-6.748	3.000e-06	0.00746	0.879	0.841
tsq_000_03011	CdKRu ₄ S ₃ SiSn ₄ Te	15	-4.81	-5.138	1.000e-06	0.00963	1.116	1.484
tsq_000_03066	Cs ₅ Yb ₄	9	-0.806	-0.901	-1.260e-05	0.00404	1.381	2.624
tsq_000_03076	AlBa ₂ Ni ₅ Pd ₃ SbZn	13	-4.373	-4.515	0.000e+00	0.0071	0.55	0.716
tsq_000_03080	Ge ₃ LaNbRu ₈ Si ₃	16	-7.415	-7.689	0.000e+00	0.00585	0.474	0.862
tsq_000_03099	Eu ₂ Ge ₅ Ru ₄ Sr	12	-5.474	-5.705	-2.000e-06	0.00545	0.527	3.849
tsq_000_03109	Ni ₇ Se ₈ Zn	16	-4.188	-4.393	-3.000e-05	0.00723	0.965	0.902
tsq_000_03125	Cs ₅ Yb ₄	9	-0.81	-0.903	1.400e-06	0.00274	1.74	2.545
tsq_000_03147	Dy ₄ I ₈	12	-3.462	-3.57	0.000e+00	0.00413	0.435	1.15
tsq_000_03156	Co ₈ Dy ₂ In ₅ Lu	16	-4.88	-5.161	-6.000e-06	0.00856	0.845	0.805
tsq_000_03159	Cu ₃ Dy ₂ Ni ₉	14	-4.893	-5.107	-6.300e-05	0.00713	0.778	0.623
tsq_000_03160	CsI ₉ Nd ₄	14	-3.397	-3.691	-4.000e-06	0.00655	0.543	1.621
tsq_000_03257	Cs ₂ P ₂ Ru ₄ S ₆	14	-5.047	-5.563	-1.800e-05	0.00976	0.813	1.708
tsq_000_03302	Co ₈ Hf ₈	16	-8.454	-8.682	0.000e+00	0.00805	0.392	0.985
tsq_000_03415	Co ₆ GeNa ₆ Sn	14	-3.577	-3.846	1.000e-06	0.00765	0.743	3.204
tsq_000_03429	Pd ₈ Ru ₄ SbTb ₂	15	-6.098	-6.292	-5.000e-06	0.00569	0.626	1.346
tsq_000_03438	Ca ₃ Ni ₈ Zn	12	-4.043	-4.233	-1.500e-05	0.00758	0.433	0.442
tsq_000_03480	I ₂ Ru ₄ Sn ₂ TeTl ₄	13	-4.01	-4.346	-2.000e-06	0.00758	1.047	1.792
tsq_000_03485	I ₈ Nd ₄	12	-3.546	-3.686	0.000e+00	0.00765	0.384	1.259

Table S10. The profile of generated materials with Truncated square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tsq_000_03538	Al ₇ Li ₂ Mn ₄	13	-4.622	-5.106	-1.600e-05	0.00749	1.092	2.445
tsq_000_03545	Co ₅ Dy ₆ Ga ₂ Ge ₂	15	-5.185	-5.532	4.000e-06	0.0057	0.874	1.707
tsq_000_03628	As ₃ BaNi ₇	11	-4.871	-5.117	0.000e+00	0.00798	0.749	0.723
tsq_000_03636	Ga ₈ Gd ₂ Ru ₅	15	-5.238	-5.422	6.000e-06	0.00363	0.368	0.452
tsq_000_03646	Cs ₅ Gd ₄	9	-1.594	-1.898	4.000e-06	0.00695	1.526	1.397
tsq_000_03684	Ru ₄ SbSn ₁₁	16	-4.851	-5.172	0.000e+00	0.00445	0.974	2.026
tsq_000_03715	Ge ₅ HoMn ₆ NiRh ₂	15	-6.495	-6.781	-1.000e-05	0.00864	0.61	0.703
tsq_000_03734	As ₅ Mn ₆ Ti ₃	14	-6.878	-7.384	-3.000e-05	0.00703	0.689	1.232
tsq_000_03748	Al ₇ Co ₆ Na	14	-4.694	-5.129	-8.700e-05	0.0097	1.091	3.519
tsq_000_03778	BCl ₇ Co ₄	12	-3.725	-4.229	3.700e-05	0.00957	0.836	1.133
tsq_000_03785	Mn ₄ PSeTe ₂	8	-5.354	-6.261	-5.000e-06	0.00976	1.475	2.03
tsq_000_03802	Ni ₅ Sn ₆	11	-4.312	-4.71	1.000e-06	0.00411	1.065	1.455
tsq_000_03810	Ga ₅ Lu ₂ Ni ₈ Pd	16	-4.706	-4.887	0.000e+00	0.00887	0.59	1.304
tsq_000_03816	KMn ₄ PSn ₂	8	-5.276	-5.988	1.000e-06	0.00483	1.228	2.928
tsq_000_03865	Au ₂ Ni ₄ P ₃ Sc ₃	12	-5.57	-5.913	0.000e+00	0.00758	1.059	1.305
tsq_000_03866	As ₆ EuRu ₇	14	-6.488	-6.867	4.000e-06	0.00467	1.162	1.947
tsq_000_03907	Ru ₅ Sn ₉	14	-5.386	-5.664	-4.000e-06	0.00999	0.798	2.161
tsq_000_03913	CeCo ₅ LiSi ₇	14	-5.778	-6.103	-3.500e-05	0.00933	0.997	1.81
tsq_000_03946	Fe ₄ Ni ₄ Si ₈	16	-6.055	-6.361	-2.300e-04	0.00647	0.405	1.256
tsq_000_03948	Al ₅ Ni ₄ Sb ₅	14	-4.282	-4.535	-1.500e-05	0.00898	0.924	1.339
tsq_000_03988	Fe ₅ La ₄ Ni ₂ Sb ₂ Zn	14	-5.656	-5.94	1.300e-05	0.00941	1.002	1.593
tsq_000_04004	Rb ₂ SSnTb ₄ Te ₃	11	-3.797	-4.348	1.000e-06	0.00387	1.557	3.86
tsq_000_04070	Al ₈ LiRu ₄ Ti ₂	15	-5.419	-6.088	-3.000e-06	0.00498	0.743	1.069
tsq_000_04128	Fe ₄ Na ₅ P ₃	12	-4.302	-4.583	0.000e+00	0.00698	0.737	0.749
tsq_000_04195	Cs ₅ Dy ₄	9	-1.645	-1.85	-4.000e-06	0.00505	1.758	2.542
tsq_000_04242	Ge ₅ Mn ₅ Na ₃ Sn ₂	15	-4.591	-5.094	-2.900e-05	0.00622	0.627	1.464
tsq_000_04279	HgI ₁₀ Nd ₄	15	-3.062	-3.42	-6.000e-06	0.00496	0.543	1.528
tsq_000_04294	Co ₄ Sb ₈ V	13	-5.114	-5.369	2.000e-06	0.00539	0.59	0.661
tsq_000_04349	Er ₇ Fe ₈ Sn	16	-5.924	-6.262	-3.000e-05	0.00831	0.908	1.194
tsq_000_04371	Ga ₁₂ Mn ₄	16	-4.03	-4.352	1.000e-06	0.00568	1.011	1.748
tsq_000_04381	Al ₆ Ru ₈ SbSc	16	-6.578	-6.855	0.000e+00	0.00699	0.379	0.515
tsq_000_04410	Ce ₉ GaSbTb ₄ Tl	16	-4.96	-5.158	5.000e-06	0.00865	0.644	0.821
tsq_000_04432	Al ₇ Ce ₂ Fe ₇	16	-5.739	-6.054	2.000e-06	0.00667	0.966	2.392
tsq_000_04452	Co ₇ Ge ₂ In ₃ La ₃	15	-5.268	-5.496	-2.000e-06	0.00735	0.538	1.563
tsq_000_04454	AgAl ₄ Ce ₅ Ge ₂ Ru ₄	16	-5.803	-6.12	-1.000e-06	0.00428	0.85	1.356
tsq_000_04469	DyGaLa ₃ Ru ₈ Ti	14	-7.083	-7.456	0.000e+00	0.00649	0.833	0.918
tsq_000_04495	Al ₃ Co ₅ Ho ₃ MnNi ₂	14	-5.62	-5.887	-3.000e-06	0.00823	0.789	1.017
tsq_000_04505	Ga ₄ La ₃ Ni ₅ Sb	13	-4.505	-4.848	0.000e+00	0.00575	0.889	1.094
tsq_000_04574	GaGdLi ₃ Ru ₄ S ₅	14	-5.025	-5.623	-2.100e-05	0.00588	1.407	1.562
tsq_000_04597	Ni ₆ Sn ₆	12	-4.134	-4.816	2.000e-06	0.00579	0.936	3.198
tsq_000_04664	Al ₄ Co ₆ PrYb	12	-5.083	-5.448	-1.400e-05	0.00703	0.524	0.819
tsq_000_04669	Ni ₅ SeTe ₃ Tl ₃	12	-3.814	-4.041	-1.000e-05	0.0097	0.471	0.619
tsq_000_04746	I ₆ Tb ₄ Zr ₂	12	-3.911	-4.232	0.000e+00	0.00791	0.545	0.873
tsq_000_04763	Br ₆ SnTb ₄	11	-3.433	-4.141	-1.500e-05	0.00277	0.605	3.935
tsq_000_04802	GeLa ₆ Ru ₇ Sn ₂	16	-6.515	-6.83	-1.000e-05	0.00397	0.919	0.981
tsq_000_04846	FeGa ₆ LiPdRu ₄	13	-4.973	-5.491	-1.100e-05	0.00683	1.144	2.761
tsq_000_04920	Al ₅ Co ₅ Mg ₄	14	-4.097	-4.354	-1.000e-06	0.00596	0.304	0.553
tsq_000_04969	AgGe ₂ Hf ₅ Mn ₅ Ru	14	-7.973	-8.274	0.000e+00	0.00512	0.73	0.435
tsq_000_05063	Cs ₅ Dy ₄	9	-1.592	-1.857	-1.900e-05	0.00824	1.262	1.501
tsq_000_05072	BaLiMn ₄ Sn ₅	11	-4.537	-5.326	-3.500e-05	0.00854	1.63	1.637
tsq_000_05078	Ca ₅ Ni ₅ Sn ₂	12	-3.742	-3.943	6.000e-06	0.00684	0.679	0.701
tsq_000_05118	In ₃ Lu ₄ Ni ₇	14	-4.653	-4.867	-1.000e-06	0.00712	0.623	0.809

Table S10. The profile of generated materials with Truncated square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tsq_000_05125	KMn ₄ Se ₈ Zr	14	-5.47	-5.83	1.100e-05	0.00646	0.987	1.314
tsq_000_05136	Cs ₄ Gd ₄	8	-1.705	-2.173	-2.000e-06	0.00339	2.848	3.258
tsq_000_05187	Co ₄ Ga ₆ Gd ₂ K	13	-4.192	-4.391	-8.000e-06	0.00951	0.664	1.515
tsq_000_05200	La ₂ Ni ₁₀ Sn	13	-5.141	-5.359	-2.800e-05	0.0083	0.42	2.697
tsq_000_05208	Br ₇ CdSeYb ₄	13	-2.475	-3.392	0.000e+00	0.00332	2.305	2.967
tsq_000_05212	AgAl ₈ Fe ₄	13	-4.67	-5.101	-2.200e-05	0.00394	1.008	0.883
tsq_000_05291	Ru ₄ Sb ₄ Sn ₆	14	-5.14	-5.484	0.000e+00	0.00703	0.671	0.87
tsq_000_05301	Co ₅ PrSnTm ₃	10	-5.424	-5.812	4.000e-06	0.0093	0.851	0.965
tsq_000_05380	NdRu ₅ Se ₇	13	-5.666	-6.055	0.000e+00	0.00522	0.425	0.963
tsq_000_05443	K ₃ Ni ₄ Sn ₃	10	-3.376	-3.597	3.000e-06	0.00831	0.542	0.627
tsq_000_05449	Cs ₅ Yb ₄	9	-0.818	-0.901	-7.000e-07	0.00249	1.27	3.197
tsq_000_05548	Fe ₅ La ₃ Si ₈	16	-6.05	-6.482	1.000e-05	0.00594	0.387	1.356
tsq_000_05554	Co ₆ Ga ₆ La ₂	14	-4.969	-5.162	2.000e-06	0.00914	0.596	1.33
tsq_000_05555	Mn ₅ Pd ₂ Sn ₅	12	-5.511	-6.049	-2.000e-06	0.0073	1.142	1.424
tsq_000_05578	Ga ₁₂ Ru ₄	16	-4.206	-4.606	-2.000e-06	0.00966	1.322	1.557
tsq_001_00032	Cs ₄ Yb ₄	8	-0.711	-0.912	1.100e-06	0.0024	2.667	2.562
tsq_001_00065	Al ₂ Ge ₃ Mn ₄ P ₄ SrTi ₂	16	-5.793	-6.281	0.000e+00	0.00839	1.293	1.82
tsq_001_00190	BaCaFe ₄ Ga ₆ GeMnSn ₂	16	-4.466	-4.735	-6.000e-06	0.00716	0.969	2.43
tsq_001_00209	Fe ₆ PSi ₃ Sn ₅	15	-5.638	-5.921	1.000e-06	0.00555	0.458	0.601
tsq_001_00212	CuGd ₅ I ₇ Pd	14	-3.407	-3.827	-6.000e-06	0.00918	1.571	1.766
tsq_001_00227	As ₂ FeLi ₅ Ni ₅	13	-4.088	-4.31	-4.000e-06	0.00527	0.803	1.325
tsq_001_00250	Co ₄ Ge ₂ Na ₅	11	-3.468	-3.702	-9.000e-06	0.0063	1.015	1.478
tsq_001_00476	Co ₆ GeLa ₃ Pb ₄	14	-4.992	-5.461	-8.000e-06	0.00541	1.029	2.039
tsq_001_00477	Ba ₂ Ru ₄ Sn ₆	12	-5.055	-5.393	0.000e+00	0.00739	0.744	0.698
tsq_001_00564	Cs ₅ Nd ₄	9	-1.731	-1.973	-5.000e-06	0.00312	0.867	2.294
tsq_001_00656	Co ₄ Sb ₂ Zr ₇	13	-7.319	-7.678	6.000e-06	0.00848	0.642	1.609
tsq_001_00671	Cs ₅ Dy ₄ Li	10	-1.601	-1.887	0.000e+00	0.0048	1.739	3.248
tsq_001_00737	Co ₄ Ge ₂ La ₃	9	-5.832	-6.031	-7.500e-05	0.00844	0.865	0.575
tsq_001_00740	Cs ₅ Gd ₄	9	-1.624	-1.873	-6.300e-05	0.00629	1.493	1.621
tsq_001_00782	Ni ₅ Pr ₄ Sn ₅	14	-4.798	-5.059	-1.000e-05	0.00497	0.551	0.829
tsq_001_00824	PRu ₄ Sn ₄ SrTe	11	-5.204	-5.815	1.000e-06	0.00605	1.541	3.389
tsq_001_00847	Pd ₁₂ Ru ₄	16	-5.31	-6.126	-4.000e-06	0.006	0.923	1.086
tsq_001_00874	CdCs ₅ Yb ₆	12	-0.809	-1.005	-6.800e-05	0.00597	2.593	3.642
tsq_001_00893	Fe ₅ Li ₉	14	-3.46	-3.837	0.000e+00	0.00852	0.915	1.033
tsq_001_00925	CeGe ₇ PdRu ₅	14	-6.133	-6.581	-1.100e-05	0.00869	0.713	1.611
tsq_001_00962	AsMn ₅ RbSe ₄ Te	12	-5.374	-5.854	-2.000e-06	0.00702	1.074	1.35
tsq_001_01007	Co ₆ Sn ₅ Sr ₃	14	-4.374	-4.747	-2.000e-05	0.00816	1.02	1.598
tsq_001_01039	Mn ₄ Se ₈	12	-5.246	-5.48	0.000e+00	0.00777	0.433	0.463
tsq_001_01052	GeLa ₃ Ni ₇ SbSn ₄	16	-4.898	-5.196	-3.000e-06	0.00751	0.871	1.724
tsq_001_01128	Ba ₂ Ga ₃ Ni ₄	9	-3.766	-4.026	-1.000e-06	0.00659	0.874	1.416
tsq_001_01140	Cs ₄ RbYb ₄	9	-0.792	-0.907	3.200e-06	0.00203	1.375	3.086
tsq_001_01227	Co ₆ Ge ₄ La ₂	12	-5.759	-6.072	5.000e-06	0.00803	0.827	0.905
tsq_001_01309	Cd ₂ Nd ₈ Sb ₄ Sn ₂	16	-4.084	-4.53	1.000e-06	0.00471	0.998	1.997
tsq_001_01322	Ca ₄ Ru ₇ Si ₅	16	-6.242	-6.498	0.000e+00	0.0055	0.478	0.485
tsq_001_01432	Fe ₄ Si ₆ Ti ₄	14	-6.691	-7.254	-1.000e-05	0.00391	0.961	0.79
tsq_001_01438	ClI ₃ Mn ₄	8	-4.273	-5.209	-1.900e-05	0.00674	1.661	2.089
tsq_001_01601	Al ₇ Fe ₄ LaY	13	-5.215	-5.557	-3.400e-05	0.00756	0.746	0.882
tsq_001_01603	As ₄ B ₂ LaLiNi ₅ Sr ₂	15	-4.829	-5.115	-3.000e-06	0.00936	1.065	2.378
tsq_001_01680	Al ₄ Eu ₂ Ni ₄ P ₂	12	-4.468	-4.971	-1.300e-05	0.00976	1.448	1.419
tsq_001_01688	Cs ₄ Sn ₂ Yb ₅	11	-1.496	-1.738	0.000e+00	0.00271	1.666	1.99
tsq_001_01701	Ca ₂ ErFe ₅ Sn ₈	16	-4.587	-4.956	-4.000e-06	0.00392	0.661	0.95
tsq_001_01745	KRu ₄ Sb ₃ Sn ₂	10	-5.133	-5.645	-1.000e-06	0.00905	1.7	1.745

Table S10. The profile of generated materials with Truncated square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tsq_001_01756	Ga ₅ Ho ₄ Ru ₅	14	-5.549	-5.935	-1.000e-06	0.00792	0.84	1.382
tsq_001_01767	Ca ₃ Ga ₂ GeMn ₄ NiSi ₂	13	-4.868	-5.369	-2.000e-06	0.00901	0.668	2.239
tsq_001_01880	Cs ₅ Nd ₄	9	-1.717	-2.002	-1.000e-05	0.00364	1.341	1.343
tsq_001_01928	Cs ₄ Tb ₄	8	-1.742	-2.155	6.000e-06	0.00911	2.726	3.124
tsq_001_01947	Ga ₉ Mn ₅ Sr	15	-4.54	-4.796	-1.000e-06	0.00789	0.644	0.883
tsq_001_02026	CsGd ₅ I ₇ Se	14	-3.445	-3.735	-4.000e-06	0.00558	1.144	1.828
tsq_001_02055	Ba ₃ Ge ₂ Mn ₅ NdSn ₅	16	-4.96	-5.149	-6.000e-06	0.00706	0.49	1.525
tsq_001_02136	Ni ₈ Sn ₅ Ti	14	-4.93	-5.136	2.300e-05	0.00999	0.433	0.516
tsq_001_02151	Li ₂ NiRu ₇ Sn ₅	15	-5.858	-6.089	-1.000e-05	0.00917	0.87	0.831
tsq_001_02233	Cd ₁₀ GaRu ₄	15	-2.714	-2.926	0.000e+00	0.00443	0.342	0.874
tsq_001_02236	GeLa ₂ Nd ₃ Ru ₈ Si	15	-6.968	-7.264	0.000e+00	0.00812	0.86	0.951
tsq_001_02241	KRu ₄ Sn ₄	9	-5.014	-5.66	-2.000e-06	0.00588	0.794	0.782
tsq_001_02242	Cs ₅ Yb ₄	9	-0.679	-0.902	1.000e-07	0.00226	1.025	3.372
tsq_001_02259	Co ₃ ErGa ₅ Mn ₆ Sn	16	-5.779	-6.088	1.000e-06	0.00979	0.635	2.627
tsq_001_02382	Ru ₄ Se ₄	8	-5.273	-6.127	0.000e+00	0.0062	1.283	1.899
tsq_001_02417	Co ₅ Ga ₆ PrSr ₂	14	-4.105	-4.472	-1.000e-06	0.00683	0.881	1.315
tsq_001_02496	Br ₆ Fe ₆	12	-4.324	-4.731	-5.000e-06	0.00626	0.657	1.84
tsq_001_02541	Al ₃ Ce ₆ Ru ₇	16	-7.139	-7.324	0.000e+00	0.00684	0.302	1.0
tsq_001_02542	Cs ₅ Yb ₄	9	-0.776	-0.898	-1.040e-05	0.00179	1.487	1.673
tsq_001_02544	Co ₄ LiSn ₇	12	-4.351	-4.684	-1.000e-06	0.00435	0.916	0.884
tsq_001_02579	Ce ₂ Co ₅ Ga ₉	16	-4.598	-4.86	3.000e-06	0.00807	0.744	1.063
tsq_001_02753	Fe ₅ Hf ₄ SbSi ₅ Ta	16	-7.603	-8.117	1.000e-05	0.00988	1.614	2.615
tsq_001_02777	Co ₅ MgTe ₉ Tl	16	-3.996	-4.241	8.000e-06	0.00998	0.554	0.797
tsq_001_02849	Co ₆ Ga ₇ Y	14	-4.843	-5.095	-2.000e-06	0.00533	0.919	0.72
tsq_001_02895	Ba ₃ Ru ₆ Si ₅ Sn	15	-5.918	-6.306	-1.000e-06	0.00396	0.697	1.769
tsq_001_03017	CdCo ₈ Er ₂ Ge ₅	16	-5.343	-5.723	-2.000e-05	0.00917	0.876	1.795
tsq_001_03026	Ge ₁₀ Mn ₆	16	-5.515	-6.035	-2.000e-06	0.0085	1.275	2.564
tsq_001_03083	FeGeMn ₇ ReSi ₅ Ti	16	-7.725	-7.752	0.000e+00	0.00683	0.678	2.254
tsq_001_03153	AlGaLa ₂ Ni ₁₀ Sn ₂	16	-5.051	-5.152	-6.000e-06	0.00828	0.608	0.739
tsq_001_03210	As ₉ Fe ₅ Si	15	-5.553	-5.868	-7.800e-05	0.00481	1.104	1.219
tsq_001_03259	Cs ₅ Tb ₄	9	-1.655	-1.871	-2.000e-06	0.0034	1.038	1.018
tsq_001_03264	Ga ₅ La ₃ Ru ₆	14	-6.006	-6.29	-4.000e-06	0.00749	0.238	0.602
tsq_001_03278	Fe ₄ Si ₆ Zr ₆	16	-7.275	-7.756	0.000e+00	0.00555	0.64	1.122
tsq_001_03283	ErIn ₄ Nd ₂ Ru ₇ Sb ₂	16	-5.786	-6.136	-4.000e-06	0.00824	0.91	1.26
tsq_001_03428	Ge ₂ La ₄ Sb ₅ Yb ₅	16	-3.804	-4.476	1.000e-06	0.0054	0.944	2.101
tsq_001_03455	AsCl ₆ CuMn ₅	13	-4.416	-5.009	-2.400e-05	0.00528	1.139	1.598
tsq_001_03465	Ga ₂ Ho ₅ Ru ₇	14	-6.547	-6.911	0.000e+00	0.00852	0.592	2.178
tsq_001_03470	Cs ₄ Yb ₄	8	-0.749	-0.94	-3.000e-07	0.00137	2.087	1.905
tsq_001_03498	Al ₄ Fe ₄ SbZr ₅	14	-6.639	-6.928	-1.000e-06	0.00537	0.429	0.904
tsq_001_03519	Co ₄ Na ₅	9	-3.083	-3.226	2.000e-06	0.00593	0.89	1.517
tsq_001_03541	Ga ₉ KRu ₅	15	-4.653	-5.086	1.000e-06	0.00558	0.767	1.643
tsq_001_03598	Al ₆ CaDyFe ₄ Ni	13	-4.88	-5.331	-3.000e-06	0.00948	1.119	1.321
tsq_001_03640	Ga ₂ Pr ₄ Ru ₈ Si	15	-6.805	-7.155	0.000e+00	0.00436	0.945	1.988
tsq_001_03688	Fe ₄ Pr ₄ Si ₄	12	-5.923	-6.347	8.000e-06	0.00729	0.942	2.748
tsq_001_03711	BaCs ₆ NaYb ₄	12	-0.854	-1.013	-6.000e-06	0.00192	1.762	2.019
tsq_001_03713	Cs ₄ Yb ₄	8	-0.689	-0.917	-5.900e-06	0.00263	2.23	2.114
tsq_001_03727	Co ₅ Ge ₃ Pr ₄	12	-5.491	-5.913	-7.000e-06	0.00695	1.535	1.622
tsq_001_03752	Cs ₅ Yb ₄	9	-0.824	-0.9	-8.000e-07	0.00236	1.712	1.538
tsq_001_03809	Ga ₄ Gd ₂ Ni ₈	14	-4.702	-4.967	-1.100e-05	0.00753	0.912	1.173
tsq_001_03844	Co ₅ Ge ₁₀	15	-4.939	-5.328	-1.000e-06	0.00898	0.774	1.16
tsq_001_03845	CeFe ₄ Ga ₁₀ Nd	16	-4.481	-4.676	-1.000e-05	0.00655	0.658	0.896
tsq_001_03873	Ca ₄ Ru ₄ Sb ₇ Sn	16	-4.868	-5.111	-2.000e-06	0.00493	0.683	0.685

Table S10. The profile of generated materials with Truncated square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tsq_001_03874	Dy ₄ I ₈ Na ₂ O ₈	15	-3.595	-3.881	-2.900e-05	0.00772	0.589	1.124
tsq_001_03920	As ₄ Co ₄ La ₂	10	-5.659	-5.993	-4.400e-05	0.00923	0.97	1.083
tsq_001_03947	CaRu ₄ Sn ₁₀	15	-4.515	-5.176	-1.000e-06	0.00592	1.548	1.613
tsq_001_04136	Al ₆ AuGeMn ₅ Nd ₂	15	-5.341	-5.756	-4.000e-06	0.00841	0.873	2.308
tsq_001_04180	Co ₄ NiSi ₃ SnZr ₅	14	-6.883	-7.282	-1.000e-05	0.00775	0.883	1.206
tsq_001_04220	Gd ₃ Ru ₄ Si ₂	9	-6.563	-7.303	-5.300e-05	0.0058	0.715	2.86
tsq_001_04243	Ge ₂ Ru ₄ S ₆	12	-5.504	-6.075	-3.000e-06	0.00468	0.172	2.722
tsq_001_04259	Ni ₇ Pr ₂ Sn ₅	14	-4.753	-5.108	6.000e-06	0.00536	1.494	1.89
tsq_001_04270	Co₄Na₃Sn₂	9	-3.642	-4.008	-7.000e-06	0.00931	0.989	0.693
tsq_001_04309	Br ₁₀ Yb ₄ Zr ₂	16	-3.479	-3.836	-3.000e-06	0.00393	1.248	2.857
tsq_001_04347	Fe₄Ga₉Li₂Y	16	-4.151	-4.344	-2.000e-06	0.0047	0.606	0.869
tsq_001_04353	BaCa₂Ni₅P₂Se₆	16	-4.499	-4.724	-6.000e-06	0.0098	0.477	0.618
tsq_001_04356	Cs ₅ Na ₆ Yb ₄	15	-0.99	-1.096	3.500e-05	0.00663	1.454	2.769
tsq_001_04390	Cs ₅ Yb ₄	9	-0.808	-0.906	-7.700e-06	0.00186	1.122	1.333
tsq_001_04400	Ni₅Sn₇Sr₃	15	-4.031	-4.166	3.000e-06	0.00725	0.22	0.931
tsq_001_04452	LaNi ₄ Se ₇	12	-4.522	-4.82	-3.100e-05	0.00759	1.448	2.536
tsq_001_04487	Fe ₄ Ga ₇ GeSc	13	-4.575	-4.998	1.000e-06	0.00435	0.515	1.295
tsq_001_04501	Co ₈ La ₂ Si ₆	16	-6.232	-6.546	1.000e-05	0.00705	0.608	1.39
tsq_001_04564	Co ₈ Ge ₃ Nd ₂ Sc	14	-5.695	-6.235	2.000e-06	0.00562	1.045	1.051
tsq_001_04588	Ni ₄ P ₂ Sn ₃	9	-4.681	-5.056	0.000e+00	0.00523	1.026	1.538
tsq_001_04705	Cs ₆ Yb ₄	10	-0.718	-0.901	-1.520e-05	0.00209	1.476	2.101
tsq_001_04721	Fe ₆ NdSi ₇	14	-6.415	-6.852	-1.900e-05	0.00632	0.475	1.312
tsq_001_04790	As ₅ CuFe ₅ Si ₂ V	14	-5.984	-6.313	2.000e-06	0.00877	0.394	1.069
tsq_001_04816	Ga₄Ni₄Sr₃	11	-3.478	-3.673	-1.600e-05	0.00893	0.639	0.504
tsq_001_04826	Cs ₅ Yb ₅	10	-0.798	-0.956	1.000e-07	0.00268	1.675	2.271
tsq_001_04839	CaCdMn ₄ Se ₇	13	-4.912	-5.239	-1.400e-05	0.00941	0.634	1.088
tsq_001_04869	Co ₇ Pr ₂ Sn ₇	16	-5.222	-5.399	0.000e+00	0.00681	0.654	1.224
tsq_001_04880	Bi ₂ GeI ₃ LaNi ₅ S ₂ Sb	15	-4.095	-4.453	-3.000e-06	0.00701	1.427	1.862
tsq_001_04890	Cs ₄ SbYb ₄	9	-1.291	-1.498	-2.900e-05	0.00305	2.349	4.226
tsq_001_04893	Cs ₃ K ₃ Yb ₄	10	-0.818	-0.961	-4.070e-05	0.00285	1.244	1.907
tsq_001_04896	Co₇Ge₇	14	-5.483	-5.754	6.000e-06	0.00905	1.161	0.867
tsq_001_04999	GdPr ₂ Ru ₅ SbSn ₆	15	-5.747	-6.066	-6.000e-06	0.00436	0.829	1.298
tsq_001_05045	Cs ₄ RbYb ₄	9	-0.804	-0.9	-3.400e-06	0.00403	1.166	2.209
tsq_001_05051	ErNi ₇ Sn ₈	16	-4.212	-4.765	-1.000e-06	0.00792	1.039	2.014
tsq_001_05103	NbRu₅Se₈	14	-5.94	-6.249	-4.000e-06	0.00812	1.034	0.656
tsq_001_05179	GaN₄Ni₄	9	-2.938	-3.158	0.000e+00	0.00692	0.932	0.846
tsq_001_05197	EuMn ₅ P ₅ Sn ₃	14	-5.88	-6.335	-1.000e-06	0.00877	0.837	1.245
tsq_001_05224	Co₄Ga₆Na₆	16	-3.09	-3.252	-2.000e-06	0.00686	0.583	0.798
tsq_001_05255	Cs ₅ Nd ₄	9	-1.709	-2.001	-1.000e-06	0.00282	1.379	1.532
tsq_001_05348	Co ₄ Sn ₅	9	-4.604	-5.18	-3.000e-06	0.00761	1.185	2.005
tsq_001_05368	Al ₆ Ni ₆ PSr ₃	16	-4.136	-4.446	-2.000e-05	0.009	1.085	1.773
tsq_001_05400	Fe ₄ Na ₅ P	10	-3.758	-4.109	-1.000e-06	0.00341	1.237	2.383
tsq_001_05474	I ₄ Ru ₄	8	-4.363	-4.934	-4.000e-06	0.00861	0.982	1.002
tsq_001_05537	La ₆ Sb ₆ Tb ₄	16	-5.026	-5.259	-3.000e-06	0.0068	0.505	1.151
tsq_001_05580	Al ₈ Fe ₅	13	-4.981	-5.494	-4.300e-05	0.00674	0.861	1.027
tsq_001_05607	Al ₃ GeLaNi ₆ Si	12	-4.918	-5.332	-1.100e-05	0.00669	0.898	2.493
tsq_001_05651	CoFe ₆ Si ₅ Tb ₄	16	-6.357	-6.643	0.000e+00	0.00556	0.883	1.271
tsq_001_05680	Co ₄ La ₂ LiSb ₂ Sm	10	-5.186	-5.493	0.000e+00	0.00976	0.937	1.003
tsq_002_00022	Al ₃ Co ₄ Ni ₃ SbSn ₂	13	-5.004	-5.296	-1.400e-05	0.00793	1.061	1.616
tsq_002_00062	Nd ₇ Sn ₇	14	-4.428	-4.958	-1.000e-06	0.0042	1.881	2.273
tsq_002_00128	Cs ₅ Nd ₄	9	-1.719	-2.004	7.000e-06	0.00521	1.422	1.754
tsq_002_00133	CaCs ₅ Yb ₆	12	-0.881	-1.034	-9.000e-06	0.00129	1.585	1.887

Table S10. The profile of generated materials with Truncated square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tsq_002_00138	GaGePRu ₈ SiSnSr	14	-6.671	-6.991	-4.000e-06	0.0065	0.563	1.095
tsq_002_00198	Co ₅ Ga ₂ Pt ₈	15	-5.889	-6.069	-3.000e-06	0.00963	0.156	0.684
tsq_002_00213	Ca ₇ Ru ₆	13	-4.667	-5.128	0.000e+00	0.008	1.885	4.196
tsq_002_00293	Se ₈ Tb ₄	12	-4.616	-5.243	-1.000e-06	0.00497	2.153	3.194
tsq_002_00335	AgBiCdSbSn ₇ Tb ₄	15	-3.798	-4.155	-7.000e-06	0.005	2.006	2.229
tsq_002_00357	Co ₆ GeSb ₆ Sn ₂	15	-4.668	-5.239	-1.000e-06	0.0071	0.902	1.106
tsq_002_00440	Co ₅ P ₈ Tc	14	-6.145	-6.605	-4.000e-06	0.00741	1.269	1.28
tsq_002_00477	Ga ₈ Ru ₄ Zr ₄	16	-5.822	-6.356	-1.000e-05	0.00605	1.308	2.485
tsq_002_00520	CsI ₆ Nd ₄ Sb	12	-2.933	-3.832	-4.000e-06	0.0059	2.269	2.931
tsq_002_00525	Gd ₃ LiRu ₉ U	14	-7.357	-7.825	1.000e-05	0.00622	0.726	0.862
tsq_002_00613	NaNi ₉ Sn ₄	14	-4.477	-4.733	-3.200e-05	0.00875	0.306	0.788
tsq_002_00674	Ru ₇ Sn ₉	16	-5.79	-6.088	0.000e+00	0.00433	0.64	1.028
tsq_002_00691	Al ₂ Co ₄ Dy ₂ Ga ₄ Ge	13	-4.704	-5.009	-3.000e-06	0.00879	0.732	0.702
tsq_002_00698	Co ₄ Ge ₉ V ₃	16	-5.554	-5.995	3.000e-06	0.00849	0.89	1.868
tsq_002_00738	CaGe ₆ Mn ₇ Sr	15	-5.823	-6.273	1.000e-06	0.00888	0.796	1.021
tsq_002_00758	La ₃ Ni ₅	8	-5.085	-5.484	-7.000e-06	0.00886	0.751	2.774
tsq_002_00768	Ca ₂ Ni ₅ Sn ₅	12	-4.102	-4.376	-3.000e-06	0.00722	1.041	0.764
tsq_002_00776	Cs ₄ Yb ₄	8	-0.717	-0.876	1.300e-06	0.00203	1.542	1.392
tsq_002_00784	Co ₆ Se ₅ Sn ₂	13	-4.894	-5.238	-4.000e-05	0.0079	1.254	2.228
tsq_002_00801	Mn ₄ Se ₃ Si	8	-5.537	-6.46	-1.000e-06	0.00347	1.335	4.256
tsq_002_00850	Cs ₅ Gd ₄	9	-1.678	-2.008	-1.000e-05	0.00204	3.067	2.976
tsq_002_00963	BrGe ₂ K ₂ LaRu ₄	10	-5.077	-5.513	-1.000e-06	0.00629	1.492	1.247
tsq_002_00977	Cs ₅ Yb ₄	9	-0.753	-0.907	-7.100e-06	0.00231	2.179	3.15
tsq_002_01014	Al ₅ Ni ₆ Sm ₂	13	-4.775	-5.104	-3.600e-05	0.00677	0.688	1.141
tsq_002_01028	Ge ₅ Ru ₄ Sn ₃ Sr	13	-5.186	-5.675	-2.000e-06	0.00919	1.03	1.389
tsq_002_01085	As ₅ Au ₂ CdFe ₄	12	-4.835	-5.094	0.000e+00	0.00634	0.504	0.79
tsq_002_01091	Bi ₂ HoPaRh ₂ Sb ₄ Tb ₄	14	-4.924	-5.585	-5.800e-05	0.00741	0.925	2.488
tsq_002_01139	Co ₄ Sn ₈	12	-4.439	-4.823	-1.800e-05	0.00987	1.063	3.137
tsq_002_01188	Co ₅ CuSbSe ₈	15	-4.601	-4.883	-1.100e-05	0.00732	1.114	1.583
tsq_002_01239	Ru ₄ Sn ₁₀ SrTl	16	-4.62	-4.986	-4.000e-06	0.0069	1.073	1.403
tsq_002_01272	Cs ₅ Gd ₄	9	-1.51	-1.899	1.800e-05	0.00906	1.439	1.182
tsq_002_01301	Ag ₂ CdCl ₈ Co ₄	15	-3.297	-3.484	-1.700e-05	0.00796	0.897	1.818
tsq_002_01393	Co ₄ Eu ₅ Ge ₃	12	-4.395	-4.545	1.000e-06	0.00737	0.623	0.598
tsq_002_01405	AgGeNi ₆ SSb ₃ SnU	14	-4.972	-5.241	-6.000e-06	0.00749	0.745	1.392
tsq_002_01444	Gd ₄ Ge ₆ La ₆	16	-5.01	-5.325	2.000e-06	0.00857	1.13	2.449
tsq_002_01466	AlFe ₅ Si ₆ Sr	13	-5.585	-6.248	-9.000e-06	0.00976	0.498	2.109
tsq_002_01478	Ge ₁₀ Mn ₄ Si ₂	16	-5.135	-5.575	2.000e-06	0.00809	0.583	1.495
tsq_002_01537	GeNi ₄ Sb ₅ U ₂	12	-5.675	-5.918	0.000e+00	0.00486	0.528	1.321
tsq_002_01540	NaNi ₄ Sn ₄	9	-3.94	-4.299	-1.000e-06	0.00907	0.659	2.293
tsq_002_01545	Ce ₃ Ga ₇ Ni ₄	14	-4.543	-4.714	-9.000e-06	0.00541	0.25	1.696
tsq_002_01571	Al ₅ La ₄ Ni ₄	13	-4.775	-4.967	2.000e-06	0.0092	0.631	1.444
tsq_002_01581	Cs ₄ Yb ₄	8	-0.719	-0.914	-1.870e-05	0.00184	1.428	1.855
tsq_002_01600	Ga ₉ Mn ₄ Ti ₃	16	-5.125	-5.425	-4.300e-05	0.00545	0.797	1.739
tsq_002_01623	GeMn ₅ Se ₆ Te ₂	14	-5.035	-5.574	-2.000e-06	0.00846	1.0	0.84
tsq_002_01715	BaGe ₂ La ₂ Ni ₄	9	-4.818	-5.086	-5.000e-06	0.00953	0.655	0.742
tsq_002_01767	Co ₇ Zr ₇	14	-7.652	-7.861	-1.000e-05	0.00905	0.638	1.497
tsq_002_01787	Cs ₅ Dy ₄	9	-1.6	-1.855	-4.000e-06	0.00454	1.74	1.567
tsq_002_01821	Ru ₄ Sn ₈ Sr ₃	15	-4.592	-4.919	2.000e-06	0.00531	1.0	1.773
tsq_002_01832	Ni ₆ ScSn ₈	15	-4.558	-4.786	0.000e+00	0.0092	0.814	1.323
tsq_002_01840	Cs ₄ Yb ₄	8	-0.754	-0.935	4.000e-07	0.00238	3.119	2.19
tsq_002_01846	Cs ₅ SbYb ₄	10	-1.265	-1.427	-1.000e-06	0.00328	1.808	3.297
tsq_002_01855	K ₂ Mn ₅ Se ₆	13	-5.049	-5.558	0.000e+00	0.00991	0.973	1.795

Table S10. The profile of generated materials with Truncated square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tsq_002_01865	Ca ₂ LiNi ₅ Sn ₅	13	-3.966	-4.305	-2.000e-06	0.00821	1.052	1.966
tsq_002_01937	Cs ₅ Tb ₄	9	-1.685	-1.87	-1.000e-06	0.00439	0.836	1.051
tsq_002_01982	Ba ₂ Ru ₄ Sn ₅	11	-5.241	-5.413	-8.000e-06	0.00633	0.809	1.406
tsq_002_02030	Ni ₄ Se ₄	8	-4.165	-4.541	-2.300e-05	0.00961	1.003	2.397
tsq_002_02039	As ₄ BaCo ₅ LaSb	12	-5.388	-5.685	7.000e-06	0.00964	0.913	1.196
tsq_002_02087	Cs ₈ Yb ₆	14	-0.748	-0.91	-7.300e-05	0.00463	2.294	2.568
tsq_002_02139	Ru ₄ Sn ₉	13	-5.086	-5.515	-2.000e-06	0.00594	0.766	2.863
tsq_002_02147	GaNdNi ₅ PuSi ₆ SnU	16	-5.824	-6.317	-2.000e-05	0.00765	1.073	1.511
tsq_002_02188	Pr ₅ Ru ₄ Sn ₅	14	-5.492	-5.949	-3.000e-06	0.00532	1.047	1.063
tsq_002_02237	Al ₇ Fe ₄ Ta ₃	14	-6.303	-6.794	-2.500e-05	0.00836	1.209	1.324
tsq_002_02270	Co ₇ Nd ₂ Sn ₇	16	-5.175	-5.342	-2.000e-06	0.00854	0.424	0.675
tsq_002_02285	CuEuGePbSn ₆ Sr ₂ Tb ₄	16	-3.713	-4.049	-3.000e-06	0.00479	0.751	1.004
tsq_002_02286	Ge ₅ Ru ₆ Sm ₅	16	-6.304	-6.702	0.000e+00	0.00998	1.142	2.326
tsq_002_02389	K ₂ PdRu ₄ Se ₈	15	-5.047	-5.191	5.000e-06	0.00937	0.547	0.601
tsq_002_02519	Mn ₅ Pd ₉	14	-5.966	-6.412	-2.300e-05	0.00841	1.048	1.694
tsq_002_02643	Ge ₈ MnRu ₇	16	-6.493	-6.835	0.000e+00	0.00868	1.354	0.999
tsq_002_02696	CeCo ₅ GeLiMn ₆ Si ₂	16	-6.731	-7.054	0.000e+00	0.00617	0.714	0.863
tsq_002_02717	AlGe ₆ Ni ₅ Sm	13	-4.723	-5.106	-6.000e-06	0.00634	0.703	0.962
tsq_002_02759	Cs ₄ RbTb ₄	9	-1.619	-1.892	-3.000e-06	0.00604	1.182	2.613
tsq_002_02765	Cs ₃ Sn ₂ Yb ₄	9	-1.387	-1.885	-5.000e-06	0.00371	2.207	2.902
tsq_002_02814	ClGeNa ₆ PRu ₅	14	-4.149	-4.604	-1.000e-06	0.0044	1.144	2.755
tsq_002_02817	Cd ₂ Ge ₄ Ru ₆	12	-5.646	-6.04	-1.000e-06	0.00686	1.005	1.41
tsq_002_02836	Co ₅ Pr ₂ Sn ₇	14	-4.894	-5.227	-7.000e-06	0.00811	0.81	0.879
tsq_002_02866	Ce ₉ Fe ₆ Pb	16	-6.525	-6.686	0.000e+00	0.00897	0.647	1.303
tsq_002_02872	CaCdCs ₆ Yb ₄	12	-0.835	-0.987	-1.000e-06	0.0024	1.15	3.001
tsq_002_02884	Ge ₇ Ru ₆ Y	14	-6.251	-6.802	1.000e-06	0.00504	0.601	0.705
tsq_002_02899	Cl ₁₀ Os ₂ Tb ₄	16	-3.605	-5.061	-2.000e-06	0.0072	1.932	2.652
tsq_002_02901	Co ₅ CuSe ₈	14	-4.734	-5.005	-4.400e-05	0.00775	0.858	1.444
tsq_002_02908	Co ₄ Ga ₈	12	-4.026	-4.384	4.000e-06	0.0064	0.808	2.164
tsq_002_02914	PrRh ₂ Ru ₄ Sn ₇ Ti	15	-5.925	-6.265	-6.000e-06	0.00481	0.689	1.369
tsq_002_02962	BaNd ₄ Sn ₄ Sr ₃ Tl ₄	16	-3.204	-3.406	1.000e-06	0.00568	1.024	1.653
tsq_002_02963	Co ₄ SiTe ₈	13	-4.341	-4.54	8.000e-06	0.00489	0.816	2.188
tsq_002_02978	GeMn ₄ NiSn ₁₀	16	-4.721	-5.126	0.000e+00	0.0069	0.516	1.359
tsq_002_03035	CuFe ₅ I ₉ Y	16	-3.778	-4.084	-1.900e-05	0.00897	1.068	1.569
tsq_002_03151	Cs ₅ Yb ₄	9	-0.78	-0.905	-1.300e-06	0.00304	1.819	1.569
tsq_002_03156	As ₈ Mn ₄ Ni	13	-5.734	-6.041	-1.000e-06	0.00988	0.909	0.931
tsq_002_03199	Co ₆ Eu ₆	12	-3.987	-4.32	-1.000e-06	0.00817	1.471	1.903
tsq_002_03253	Ni ₆ P ₄ SiSn	12	-5.232	-5.519	-1.000e-05	0.00797	0.476	0.607
tsq_002_03306	Co ₆ SbZr ₅	12	-7.267	-7.646	-3.000e-06	0.00731	0.6	1.6
tsq_002_03391	Cl ₄ Mn ₄	8	-4.683	-5.35	-6.000e-06	0.00647	1.144	1.478
tsq_002_03392	Ce ₇ Ge ₃ Ru ₄ SbSn	16	-6.291	-6.718	-2.000e-05	0.00499	0.831	1.125
tsq_002_03396	Cs ₅ Yb ₄	9	-0.797	-0.909	2.000e-07	0.00156	1.346	1.475
tsq_002_03446	As ₄ Na ₆ Ni ₆	16	-3.625	-3.826	0.000e+00	0.00619	1.014	2.399
tsq_002_03520	Ru ₈ Sn ₈	16	-6.017	-6.397	-2.000e-05	0.00756	0.637	0.842
tsq_002_03542	Co ₈ Ge ₃ P ₅	16	-5.92	-6.261	0.000e+00	0.00959	0.467	1.571
tsq_002_03578	Cs ₄ Yb ₄	8	-0.747	-0.876	-2.000e-07	0.00183	1.854	2.99
tsq_002_03727	Co ₄ Sn ₈	12	-4.547	-4.835	-6.000e-06	0.00514	0.513	0.842
tsq_002_03790	La ₈ Ru ₆ Sn	15	-6.447	-6.702	0.000e+00	0.008	0.316	0.815
tsq_002_03806	Co ₁₀ Ge ₃ Nd ₃	16	-5.987	-6.242	0.000e+00	0.00804	0.725	0.769
tsq_002_03810	Fe ₄ Ga ₆ Pd ₂ Y ₂	14	-5.195	-5.536	1.000e-06	0.00329	0.571	0.751
tsq_002_03858	Cs ₈ Yb ₅	13	-0.786	-0.929	3.100e-05	0.00646	1.791	3.127
tsq_002_03883	AlGe ₂ La ₅ Ru ₆	14	-6.502	-6.9	-3.000e-06	0.00936	1.0	3.575

Table S10. The profile of generated materials with Truncated square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tsq_002_03894	Ni ₄ P ₂ SSe ₅	12	-4.017	-4.603	-3.700e-05	0.00655	1.723	2.283
tsq_002_03917	Cs ₅ Yb ₄	9	-0.788	-0.902	-6.800e-06	0.00278	1.483	3.462
tsq_002_03953	Co ₇ Zr ₇	14	-7.612	-7.979	0.000e+00	0.00864	1.002	1.333
tsq_002_03965	Ga ₈ Gd ₃ Ru ₄	15	-4.84	-5.207	-4.000e-06	0.00463	0.728	1.882
tsq_002_04006	Na ₅ Ni ₄	9	-2.594	-2.787	0.000e+00	0.00507	0.601	1.127
tsq_002_04037	GeRu ₆ Se ₇	14	-5.636	-5.97	2.000e-06	0.00443	0.358	1.603
tsq_002_04111	Cs ₈ Dy ₄	12	-1.383	-1.602	-9.000e-06	0.00341	1.355	1.756
tsq_002_04132	Ru ₄ Se ₆	10	-5.427	-5.943	-6.000e-06	0.00967	1.055	1.371
tsq_002_04148	Co ₄ GePSe ₂ Sn	9	-4.956	-5.465	-3.100e-05	0.00926	0.598	2.579
tsq_002_04176	Br ₂ Dy ₄ RhSe ₆	13	-4.691	-5.214	-1.000e-05	0.00627	1.407	2.339
tsq_002_04178	Li ₂ Mg ₃ Ni ₅ SbSi ₂ Sn ₂	15	-3.621	-4.114	0.000e+00	0.00742	0.402	1.404
tsq_002_04189	Ru ₅ Sn ₁₀	15	-5.121	-5.591	-4.000e-06	0.00391	1.245	1.837
tsq_002_04224	Na ₄ Ni ₆	10	-3.217	-3.532	1.000e-06	0.00706	1.117	0.939
tsq_002_04271	As ₂ CoLi ₄ Mn ₄ Se ₂ Sn	14	-4.872	-5.233	-2.000e-06	0.00697	0.671	0.643
tsq_002_04282	Cs ₅ Yb ₄	9	-0.804	-0.909	0.000e+00	0.00236	1.499	1.812
tsq_002_04315	CsFePdRu ₄ Se ₈ Tl	16	-4.839	-5.21	-6.000e-05	0.00803	0.842	1.451
tsq_002_04347	Al ₅ CaCo ₅	11	-4.827	-5.325	-1.800e-05	0.00936	0.908	1.004
tsq_002_04350	Al ₄ Co ₄ GePr ₃	12	-5.058	-5.395	3.000e-06	0.00717	0.895	0.807
tsq_002_04390	Ge ₄ Na ₃ Ru ₆ Sn	14	-5.253	-5.641	-5.000e-06	0.0056	0.974	1.699
tsq_002_04454	As ₂ BiCo ₅ GeLa ₄	13	-5.787	-6.062	1.000e-06	0.00763	0.919	1.31
tsq_002_04455	Ga ₉ Lu ₂ Mn ₄	15	-4.544	-4.837	1.000e-06	0.0061	0.645	1.169
tsq_002_04496	GeMn ₅ Sb ₄ SrZn	12	-5.062	-5.612	-1.000e-06	0.00423	1.05	2.627
tsq_002_04505	Br ₆ ClCo ₄ PSe	13	-3.652	-3.895	-2.800e-05	0.00553	0.912	2.063
tsq_002_04591	Ge ₄ Li ₄ Ni ₅	13	-4.007	-4.252	-2.000e-06	0.00844	0.794	1.569
tsq_002_04720	Co ₅ La ₂ NiSi ₇	15	-5.864	-6.353	-1.000e-06	0.00982	0.871	1.761
tsq_002_04805	Co ₄ Eu ₂ Ge ₂	8	-4.683	-5.309	2.000e-06	0.00658	1.457	1.598
tsq_002_04863	Cs ₃ GaRu ₄ Se ₇	15	-4.46	-4.814	0.000e+00	0.00446	1.316	2.599
tsq_002_04873	MnNd ₄ SiTe ₉	15	-4.27	-4.803	1.000e-06	0.00638	1.137	2.572
tsq_002_04878	La ₃ Ni ₆ PSr	11	-5.125	-5.244	0.000e+00	0.00642	0.341	0.502
tsq_002_04964	Al ₄ Ni ₄ Sr ₄	12	-3.579	-3.837	-1.500e-05	0.00755	0.498	1.032
tsq_002_05055	AlGe ₄ Ni ₈ Th ₂	15	-5.435	-5.843	2.000e-06	0.00713	0.862	2.114
tsq_002_05058	CeLuMn ₅ Ni ₂ Si ₅ Zn	15	-6.101	-6.605	0.000e+00	0.00535	0.774	1.613
tsq_002_05119	Co ₂ Er ₂ Ge ₄ Ni ₈	16	-5.442	-5.529	2.000e-06	0.00999	0.378	0.706
tsq_002_05130	Cs ₅ Nd ₄	9	-1.708	-2.11	1.010e-04	0.00455	3.169	3.438
tsq_002_05165	MnNi ₅ Sb ₄ SiTiZr ₄	16	-6.085	-6.523	0.000e+00	0.0074	1.014	1.496
tsq_002_05284	Co ₄ EuIn ₄ La ₃ RhSb	14	-4.666	-4.963	1.100e-05	0.01	1.323	1.405
tsq_002_05305	Br ₄ Mn ₄	8	-4.352	-5.168	-1.100e-05	0.0076	1.229	1.301
tsq_002_05368	Fe ₄ Ge ₂ La ₂ PtSn ₄	13	-5.347	-5.666	-1.000e-06	0.00482	0.6	0.671
tsq_002_05409	Co ₄ K ₃ PS ₂	10	-4.29	-4.691	-2.000e-06	0.00747	1.052	1.832
tsq_002_05439	Ge ₃ Ni ₇ S ₂ Y ₂	14	-5.42	-5.637	0.000e+00	0.0056	0.697	0.791
tsq_002_05464	Br ₇ Ru ₆ S	14	-4.569	-4.929	-1.700e-05	0.00943	0.619	0.989
tsq_002_05506	La ₆ Ru ₄ Sn ₂	12	-6.242	-6.53	-1.000e-06	0.00848	0.65	0.667
tsq_002_05580	Cs ₅ Yb ₄	9	-0.73	-0.913	2.000e-07	0.00239	2.25	1.476
tsq_002_05584	Ge ₃ Ru ₄ Sb ₃ Sr ₃	13	-4.97	-5.32	-2.000e-06	0.00594	1.819	1.399
tsq_002_05635	As ₂ Co ₆ Na ₂ Se	11	-4.796	-5.209	-5.000e-06	0.00533	0.486	0.723
tsq_002_05637	Al ₂ Ge ₂ Ni ₅ Yb ₂	11	-4.38	-4.563	0.000e+00	0.00533	0.947	0.722
tsq_003_00171	Co ₅ La ₂ Sn ₃	10	-5.187	-5.572	-3.000e-06	0.00943	0.461	1.078
tsq_003_00177	Cl ₆ Mn ₄ Rb ₂	12	-4.065	-4.572	1.000e-06	0.00664	1.173	1.38
tsq_003_00215	La ₄ Ni ₉ Si	14	-5.366	-5.66	-3.700e-05	0.00817	0.775	1.872
tsq_003_00242	Ga ₇ NiPrRu ₆	15	-5.469	-5.921	-1.000e-06	0.00771	1.119	1.321
tsq_003_00256	Ce ₂ Fe ₃ Ni ₄ Si ₆	15	-6.288	-6.53	-1.900e-05	0.00738	0.445	0.94
tsq_003_00289	Ga ₇ Mn ₅ Sr ₂	14	-4.505	-4.802	1.000e-06	0.00504	0.783	1.73

Table S10. The profile of generated materials with Truncated square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tsq_003_00306	Co ₅ Sn ₈	13	-4.796	-4.968	-5.000e-06	0.00723	0.553	0.695
tsq_003_00365	Cs ₉ Tb ₄	13	-1.392	-1.533	6.600e-05	0.00724	1.06	0.861
tsq_003_00380	Eu ₅ Ge ₂ PRu ₆	14	-5.604	-5.931	-5.000e-06	0.00734	0.744	1.222
tsq_003_00383	I ₆ Ru ₄ Te	11	-3.849	-4.267	-2.000e-06	0.00641	0.569	1.492
tsq_003_00389	AlCeGa ₈ Ru ₄	14	-4.897	-5.227	3.000e-06	0.00819	0.702	1.505
tsq_003_00392	Co ₄ Ga ₇ Sr ₃	14	-3.573	-3.906	1.000e-06	0.00751	0.602	0.732
tsq_003_00491	Br ₄ Ru ₄	8	-4.29	-5.215	-4.000e-06	0.00793	1.546	1.65
tsq_003_00541	GeLa ₅ Mn ₄ Rh ₅	15	-6.574	-6.953	-2.000e-05	0.00621	1.084	2.264
tsq_003_00658	Cs ₅ Dy ₄	9	-1.657	-1.849	-4.000e-06	0.00339	0.978	1.994
tsq_003_00669	CoErGeNi ₃ PRu ₈ Si	16	-6.933	-7.392	1.000e-05	0.00556	0.62	1.549
tsq_003_00685	Cs ₅ Nd ₄	9	-1.739	-2.22	-2.600e-05	0.00996	3.114	5.504
tsq_003_00703	Fe ₄ Ga ₃ GeSn ₅	13	-4.518	-4.843	1.000e-06	0.00588	0.891	1.211
tsq_003_00727	Ru ₄ Sn ₉ Sr	14	-4.939	-5.318	-4.000e-06	0.00573	1.016	2.168
tsq_003_00757	CdNd ₄ Rb ₂ Te ₈	15	-3.71	-4.165	-4.000e-06	0.00922	2.267	3.433
tsq_003_00758	BaClKMn ₄ Se ₅	12	-4.971	-5.424	2.000e-06	0.00562	1.035	1.477
tsq_003_00832	Ga ₂ Ru ₄ Se ₈ Sr ₂	16	-4.616	-5.144	-1.000e-06	0.00596	1.048	2.654
tsq_003_00833	Co ₄ GeP ₆ Tb ₃	14	-5.953	-6.244	-8.000e-06	0.00842	0.776	0.839
tsq_003_00839	Al ₂ Ru ₅ Sn ₇	14	-5.373	-5.757	-1.000e-06	0.0058	0.396	1.093
tsq_003_00871	Cs ₅ Yb ₄	9	-0.818	-0.902	-1.500e-06	0.00307	1.098	2.221
tsq_003_00911	Ni ₅ Sn ₁₀	15	-4.211	-4.451	0.000e+00	0.00887	0.834	0.792
tsq_003_00927	Al ₈ ErRu ₅	14	-5.665	-6.197	-2.000e-06	0.0049	1.19	2.148
tsq_003_01042	Ru ₆ Sn ₅ Tl ₃	14	-5.295	-5.578	-4.000e-06	0.00719	0.485	0.618
tsq_003_01048	Eu ₂ Ga ₉ Ru ₄	15	-4.399	-4.588	2.000e-06	0.00837	0.536	0.6
tsq_003_01051	Co ₉ PY ₄	14	-6.558	-6.814	-5.300e-05	0.00839	0.707	0.61
tsq_003_01143	Ge ₃ Mn ₆ Sn ₂ Tm	12	-5.95	-6.557	-1.000e-06	0.00566	1.23	1.569
tsq_003_01213	Co ₄ P ₂ Tl ₂	8	-4.539	-5.291	-6.000e-06	0.00882	1.548	2.144
tsq_003_01243	AgCaRu ₄ S ₄ Sn ₃	13	-5.253	-5.556	-1.000e-06	0.00636	0.767	2.502
tsq_003_01287	Cs ₅ Yb ₄	9	-0.782	-0.906	-9.000e-07	0.00189	1.328	1.438
tsq_003_01327	La ₂ Ni ₆ OSn ₅	14	-4.735	-5.255	-5.000e-06	0.00751	0.971	0.815
tsq_003_01376	GaGe ₂ InNi ₈ Sm ₂	14	-4.899	-5.15	-2.000e-06	0.00898	0.707	1.54
tsq_003_01398	Co ₁₁ Y ₃	14	-6.479	-6.832	7.000e-06	0.00903	0.897	1.244
tsq_003_01399	LaNi ₅ Sb ₇	13	-4.74	-4.959	-4.000e-06	0.00639	0.732	1.074
tsq_003_01440	CeGa ₇ Mn ₄	12	-4.874	-5.245	1.000e-06	0.00956	1.229	1.745
tsq_003_01459	AlCaCo ₇ GeSbSn ₂	13	-5.082	-5.423	-4.000e-06	0.00694	1.045	0.964
tsq_003_01469	Cs ₅ Gd ₄	9	-1.478	-1.899	2.000e-06	0.00233	1.311	2.287
tsq_003_01477	Ru ₉ Sn ₇	16	-6.185	-6.656	-1.000e-05	0.00784	0.407	0.892
tsq_003_01499	Cs ₅ Dy ₄	9	-1.579	-1.857	-6.000e-06	0.00256	0.993	1.098
tsq_003_01500	Ni ₅ Sn ₈	13	-4.29	-4.573	-3.000e-06	0.00596	0.542	1.558
tsq_003_01528	Ge ₂ Ru ₄ SbSn ₆	13	-5.117	-5.554	0.000e+00	0.0062	0.695	2.453
tsq_003_01576	Ru ₄ Se ₄ Sn	9	-5.378	-5.935	8.000e-06	0.00637	0.598	0.95
tsq_003_01585	Co ₄ Ge ₃ Rb ₃	10	-3.937	-4.125	-1.000e-06	0.00685	1.087	1.57
tsq_003_01589	Cs ₄ Tb ₄	8	-1.763	-2.155	-1.300e-05	0.00622	2.546	2.355
tsq_003_01687	Ge ₄ Ni ₅ Sn ₃ Sr ₂	14	-4.248	-4.562	-4.700e-05	0.0087	0.56	1.734
tsq_003_01707	Co ₅ Dy ₂ Ga ₄ La ₂	13	-5.161	-5.298	0.000e+00	0.00707	0.736	2.068
tsq_003_01826	Ru ₄ SmSn ₇	12	-5.511	-5.805	-1.000e-06	0.00586	0.93	1.157
tsq_003_01832	Mn ₅ Se ₈ Tl ₂	15	-5.07	-5.407	1.000e-06	0.00773	0.892	0.652
tsq_003_01896	Pd ₃ Ru ₄ Sn ₉	16	-5.204	-5.499	-4.000e-06	0.00805	0.899	1.002
tsq_003_01901	Al ₆ Ni ₇ Ta	14	-5.223	-5.558	-6.000e-06	0.0089	1.218	0.773
tsq_003_01907	GaLiRu ₄ Se ₇ Si	14	-5.005	-5.242	-1.000e-06	0.00752	0.72	1.158
tsq_003_02017	Co ₄ Sn ₃ Sr ₂	9	-4.447	-4.698	3.000e-06	0.00938	0.679	0.542
tsq_003_02138	As ₃ Ca ₄ Ru ₅	12	-5.358	-5.882	-2.000e-06	0.00555	0.933	1.722
tsq_003_02143	Bi ₄ Eu ₃ Fe ₆ Sb	14	-5.008	-5.318	-1.200e-05	0.00644	1.322	2.921

Table S10. The profile of generated materials with Truncated square lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
tsq_003_02174	Ga ₂ Ru ₄ Se ₉	15	-4.755	-5.118	-5.000e-06	0.00856	0.609	2.126
tsq_003_02192	Ba ₃ Ga ₃ Ru ₄	10	-4.735	-5.063	1.000e-06	0.00736	1.099	2.106
tsq_003_02232	Al ₈ Fe ₆ Pr ₂	16	-5.254	-5.587	-7.000e-06	0.00932	0.587	0.79
tsq_003_02262	NdRu ₅ Se ₇	13	-5.699	-6.024	0.000e+00	0.0058	0.937	0.958
tsq_003_02403	Cs ₄ Yb ₄	8	-0.709	-0.919	-4.000e-07	0.002	2.161	1.833
tsq_003_02443	Cs ₂ Te ₆ Yb ₅	13	-3.014	-3.428	-8.000e-06	0.00824	1.181	4.965
tsq_003_02597	Ni ₆ Pr ₃ Sb ₅	14	-5.023	-5.254	1.000e-05	0.00982	0.778	0.946
tsq_003_02632	AsGe ₇ MoRu ₄ Ti ₃	16	-6.304	-6.874	0.000e+00	0.00692	0.925	0.945
tsq_003_02652	Fe ₆ Gd ₂ Ge ₆ Ho	15	-5.821	-6.208	-1.000e-06	0.00845	0.813	1.378
tsq_003_02718	Cs ₈ Gd ₄	12	-1.377	-1.625	-3.000e-06	0.0037	1.12	1.314
tsq_003_02752	Al ₃ Ce ₂ Ge ₄ Ni ₇	16	-5.201	-5.396	-1.200e-05	0.00802	0.781	1.83
tsq_003_02773	CoFe ₆ MgMnNiP ₄ SbSi	16	-6.265	-6.685	-5.000e-05	0.0074	1.075	1.373
tsq_003_02829	CdDyGe ₇ Ho ₂ Ru ₄ Sr	16	-5.322	-5.571	-3.000e-06	0.007	0.766	0.766
tsq_003_02873	As ₇ K ₃ Ru ₅	15	-5.301	-5.596	-4.000e-06	0.0069	0.905	0.737
tsq_003_02933	Fe ₅ Li ₇	12	-3.695	-4.216	1.000e-06	0.00523	1.579	1.464
tsq_003_02986	Ni ₄ Sb ₃ Sn	8	-4.385	-4.918	0.000e+00	0.00905	1.071	1.703
tsq_003_03010	Br ₈ GeRu ₄ Se	14	-3.47	-4.202	-5.000e-06	0.00907	1.572	2.248
tsq_003_03070	AlGe ₄ Ru ₄ SmSn ₃	13	-5.45	-5.948	0.000e+00	0.00586	1.236	1.911
tsq_003_03073	ClI ₉ Tb ₅ Te	16	-3.141	-3.862	-1.900e-05	0.00661	1.082	2.651
tsq_003_03212	BaNdRu ₄ Se ₄	10	-5.679	-6.129	-2.000e-06	0.00512	0.821	0.831
tsq_003_03302	Co ₄ S ₂ Tl ₆	12	-3.752	-3.999	-1.000e-06	0.00876	0.594	0.472
tsq_003_03317	Cs ₅ Tb ₄	9	-1.577	-1.875	-1.000e-05	0.00474	1.78	1.961
tsq_003_03380	Al ₂ BaCo ₄ P ₆	13	-5.161	-5.705	4.500e-05	0.00903	1.302	1.542
tsq_003_03430	Co ₄ FeSn ₉	14	-4.46	-4.979	1.000e-06	0.008	0.758	1.191
tsq_003_03468	Cs ₂ I ₆ SnTb ₄	13	-2.98	-3.303	-3.000e-06	0.00271	1.728	2.2
tsq_003_03533	Co ₃ GeNiRu ₈ SnTm ₂	16	-6.959	-7.286	0.000e+00	0.00959	0.648	1.29
tsq_003_03591	Al ₂ Ni ₄ Sb ₃ SnZr ₅	15	-6.021	-6.234	-1.200e-05	0.00614	0.452	1.138
tsq_003_03624	Co ₇ Sn ₄ Sr ₃	14	-4.672	-4.98	-2.000e-06	0.00908	0.962	2.033
tsq_003_03734	Cs ₅ Yb ₄	9	-0.798	-0.888	-3.000e-06	0.00232	0.924	2.183
tsq_003_03739	La ₃ Sb ₇ Tb ₆	16	-4.867	-5.314	-1.000e-06	0.00432	0.531	1.829
tsq_003_03803	Br ₈ Gd ₄	12	-3.925	-4.163	-4.000e-06	0.00304	0.977	1.909
tsq_003_03839	Ce ₂ Fe ₆ Ga ₇	15	-5.231	-5.556	0.000e+00	0.00517	0.98	1.092
tsq_003_03862	Cd ₄ Gd ₄ Te ₈	16	-3.443	-3.696	-3.000e-06	0.00478	0.303	2.872

Table S11. The profile of generated materials with Small rhombitrihexagonal lattice structures after DFT relaxation

Index	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
srt_000_00008	Ba ₄ Ru ₆ SSn ₃	14	-5.192	-5.704	-7.000e-06	0.00755	0.95	3.053
srt_000_00049	Fe ₈ Se ₈	16	-5.433	-5.956	-1.000e-06	0.00746	0.788	1.143
srt_000_00051	Al ₃ Ni ₆ Sn ₅	14	-4.58	-4.636	-1.000e-06	0.00761	0.192	0.17
srt_000_00055	Nd ₃ Ni ₁₁ Sn ₂	16	-5.081	-5.351	-1.700e-05	0.00966	1.179	1.293
srt_000_00058	Co ₆ Sn ₇	13	-4.953	-5.102	-1.000e-06	0.00943	0.362	0.469
srt_000_00062	Ni ₇ Y ₈	15	-6.048	-6.303	7.000e-06	0.00745	0.724	0.859
srt_000_00090	CeCo ₇ Sb ₂ Sn ₅	15	-5.394	-5.552	-3.000e-06	0.00757	0.159	1.161
srt_000_00094	Al ₄ AuGeMn ₁₀ Sr ₄	20	-5.304	-5.767	0.000e+00	0.00856	0.647	1.725
srt_000_00121	Ni ₆ Sn ₇	13	-4.53	-4.596	-9.000e-06	0.00631	0.437	0.497
srt_000_00245	Ba ₂ Ru ₇ Sn ₄ Sr	14	-5.8	-6.034	3.000e-06	0.00821	1.038	0.828
srt_000_00278	Ni ₆ Sn ₆	12	-4.549	-4.631	-5.800e-05	0.00866	0.458	0.783
srt_000_00405	Co ₇ Sn ₈	15	-4.985	-5.218	-8.000e-06	0.00624	0.534	0.489
srt_000_00410	GeNi ₆ Sn ₇	14	-4.404	-4.675	-8.000e-06	0.00996	0.385	0.605
srt_000_00459	AlGe ₂ Ni ₇ Rb ₂ Sb	13	-4.099	-4.401	-7.000e-06	0.00616	0.873	0.773
srt_000_00464	Cs ₈ Yb ₆	14	-0.816	-0.952	-8.000e-06	0.0023	2.052	3.236
srt_000_00587	Cs ₈ Yb ₆	14	-0.816	-0.952	-1.000e-06	0.00265	1.607	3.458
srt_000_00638	Ni ₇ Rb ₄ Sb ₄	15	-3.789	-3.937	-2.300e-05	0.00419	0.735	0.515
srt_000_00724	Mn ₇ Sn ₈	15	-5.189	-5.962	1.000e-06	0.0074	1.0	1.223
srt_000_00742	Cs ₆ Nd ₆	12	-1.99	-2.376	1.700e-05	0.00679	2.629	3.836
srt_000_00744	AlPr ₂ Ru ₉	12	-7.51	-7.891	1.000e-06	0.00845	0.439	0.463
srt_000_00772	Ni ₆ SbSn ₆	13	-4.388	-4.617	1.000e-06	0.00897	0.544	0.525
srt_000_00776	Eu ₄ Ga ₄ Ni ₆	14	-4.03	-4.158	-1.000e-06	0.00723	0.567	1.604
srt_000_00814	Co ₇ Ge ₆ Rb	14	-5.053	-5.385	-1.000e-06	0.00845	0.915	0.961
srt_000_00862	Mn ₆ Se ₄ Tl ₂	12	-5.518	-5.876	-8.000e-06	0.00518	0.607	0.5
srt_000_00881	Ni ₁₃ SbSi ₂ Sn ₄	20	-4.96	-5.195	0.000e+00	0.00857	0.801	1.608
srt_000_00886	Ga ₂ Nd ₂ Ni ₁₀ Ti	15	-5.194	-5.432	-4.000e-06	0.00517	0.659	1.025
srt_000_00934	Cs ₇ Tb ₆	13	-1.755	-2.101	-1.000e-06	0.00351	1.641	2.446
srt_000_01016	Ge ₅ Ni ₆ Rb ₂	13	-4.079	-4.414	2.000e-06	0.00726	1.175	0.926
srt_000_01029	Br ₂ Ru ₆ SSn ₄	13	-5.422	-5.804	4.000e-06	0.00841	0.25	0.949
srt_000_01106	Al ₂ Ge ₆ HoRu ₁₀	19	-6.77	-7.038	0.000e+00	0.00708	0.75	1.741
srt_000_01149	Co ₆ Ga ₅ Tl ₃	14	-4.105	-4.381	-1.750e-04	0.00641	0.363	1.988
srt_000_01199	MgNdNi ₁₁ TiU	15	-5.594	-5.852	-2.280e-04	0.00971	0.363	0.526
srt_000_01245	Fe ₆ Nd ₈	14	-5.785	-6.048	-2.600e-05	0.00458	0.639	0.707
srt_000_01280	Co ₆ La ₂ Sn ₅	13	-5.283	-5.592	-5.000e-06	0.0084	0.551	0.98
srt_000_01288	Ni ₆ Sn ₁₁	17	-4.353	-4.405	0.000e+00	0.00579	0.199	1.009
srt_000_01405	Co ₆ Dy ₂ Ga ₂ Pr ₂ Sn ₂	14	-5.36	-5.555	-3.900e-05	0.0069	0.616	0.334
srt_000_01448	Ni ₇ Sn ₅ Sr ₃	15	-4.288	-4.422	-3.700e-05	0.00653	0.897	2.198
srt_000_01491	Mn ₆ Sn ₈	14	-5.521	-5.808	-2.400e-05	0.00438	0.487	0.431
srt_000_01498	AlAsGa ₃ Ni ₆ RbY	13	-4.269	-4.557	6.000e-06	0.00654	0.726	0.8
srt_000_01501	Al ₅ Ge ₂ Ni ₇ Sm	15	-4.875	-5.063	-5.000e-06	0.0088	0.722	1.228
srt_000_01509	As ₂ Ba ₂ Ge ₂ Ru ₇ Sr ₂	15	-5.748	-6.163	-2.300e-05	0.0098	0.74	1.873
srt_000_01516	Co ₆ NdSn ₆ Sr	14	-4.797	-5.173	1.100e-05	0.00966	0.802	0.657
srt_000_01541	Ce ₃ Co ₉ GaSn ₂	15	-5.858	-6.218	-1.500e-05	0.0037	0.938	1.168
srt_000_01559	Lu ₇ Ru ₈	15	-6.494	-7.177	0.000e+00	0.00865	1.107	1.596
srt_000_01561	Cs ₈ Yb ₆	14	-0.767	-0.953	4.000e-06	0.00153	1.221	3.224
srt_000_01635	Co ₇ Ge ₃ SnZr ₅	16	-6.688	-6.991	-3.000e-05	0.00993	0.723	0.65
srt_000_01647	Cs ₉ Nd ₆	15	-1.645	-2.03	-6.100e-05	0.00158	2.404	3.361
srt_000_01657	Ru ₇ Sn ₈	15	-5.79	-6.194	-2.000e-06	0.0079	0.619	0.599
srt_000_01658	Mn ₆ SnTe ₇	14	-5.467	-5.737	-1.200e-05	0.00636	0.402	0.383
srt_000_01666	As ₂ GaLa ₂ Ru ₇ Te ₃	15	-6.085	-6.611	2.000e-06	0.00417	1.516	0.838
srt_000_01681	Cs ₆ Yb ₆	12	-0.79	-0.96	1.000e-06	0.00204	1.688	1.319
srt_000_01742	Co ₆ LiSn ₆	13	-4.801	-5.013	1.000e-06	0.00579	0.698	0.669

Table S11. The profile of generated materials with Small rhombitrihexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
srt_000_01758	Cs ₃ Ni ₆ Sn ₄	13	-3.732	-3.943	-1.000e-06	0.0076	0.783	1.49
srt_000_01796	Co ₆ SSn ₇	14	-4.975	-5.212	-1.300e-05	0.00805	0.342	0.544
srt_000_01816	CdCo ₇ GaPdPrSn ₄	15	-4.996	-5.216	-1.600e-05	0.00807	0.474	1.554
srt_000_01847	Cs ₆ Yb ₆	12	-0.784	-0.937	-1.700e-05	0.00308	1.329	2.963
srt_000_01848	Mn ₇ Sn ₇ Zr	15	-5.878	-6.322	-1.000e-06	0.00752	0.876	1.399
srt_000_01915	K ₃ Ni ₆ Sn ₅	14	-3.948	-4.012	-2.000e-06	0.00624	0.435	0.639
srt_000_01937	Co ₆ Sn ₈	14	-5.061	-5.13	-5.000e-06	0.00863	0.181	0.154
srt_000_01948	Co ₉ Sn ₁₁	20	-4.485	-5.17	0.000e+00	0.00913	1.084	1.768
srt_000_01968	La ₃ Ni ₇ Sn ₅	15	-5.088	-5.225	-5.000e-06	0.00904	0.306	0.359
srt_000_01993	Ni ₆ RbS ₇	14	-4.505	-4.818	-1.000e-06	0.00497	0.549	0.747
srt_000_02112	GeRu ₇ Si ₂ Sn ₂ Sr ₂	14	-6.197	-6.474	-2.000e-06	0.0039	0.583	0.523
srt_000_02114	La ₈ Ru ₇	15	-6.802	-7.026	-1.000e-05	0.00868	0.661	1.138
srt_000_02190	Ni ₇ SmSn ₇	15	-4.745	-4.852	-1.000e-06	0.00761	0.536	0.447
srt_000_02234	Mn ₇ Ni ₂ PdRhSn ₈	19	-5.591	-6.02	0.000e+00	0.00571	0.966	1.899
srt_000_02243	Fe ₆ Se ₆ Tl ₂	14	-5.184	-5.393	3.000e-06	0.00613	0.427	0.487
srt_000_02247	Cl ₇ ITb ₆	14	-3.203	-4.34	1.000e-06	0.0067	2.9	2.354
srt_000_02278	Fe ₆ GeLa ₄ Sn ₃	14	-6.091	-6.272	0.000e+00	0.00915	1.008	1.021
srt_000_02328	AlliNi ₆ Sn ₆	14	-4.304	-4.507	-9.000e-06	0.00522	0.405	0.434
srt_000_02399	Br ₃ Cl ₃ Mn ₆	12	-4.833	-5.342	-1.400e-05	0.00903	1.029	1.463
srt_000_02407	Co ₆ Sb ₂ Sn ₈ Sr	17	-4.798	-4.899	6.000e-06	0.0056	0.241	0.768
srt_000_02463	Mn ₆ Sn ₇	13	-5.708	-5.913	0.000e+00	0.00605	0.419	0.847
srt_000_02529	Nd ₂ Ni ₇ Sn ₆	15	-4.809	-5.025	-6.000e-06	0.00904	0.959	0.814
srt_000_02604	Co ₇ NdPrSn ₆	15	-4.795	-5.541	-7.000e-06	0.00667	1.196	1.023
srt_000_02638	Co ₆ LaSn ₇	14	-5.277	-5.34	0.000e+00	0.00917	0.35	0.434
srt_000_02643	Cs ₈ Nd ₆	14	-1.929	-2.137	0.000e+00	0.00197	1.521	2.663
srt_000_02721	Mn ₆ Sn ₇	13	-5.546	-5.897	-1.600e-05	0.00611	0.722	0.737
srt_000_02765	Co ₆ Sn ₈	14	-4.531	-5.126	-8.200e-05	0.00719	0.431	0.759
srt_000_02786	Bi ₃ Co ₆ Er ₂ Ga ₂ Y	14	-5.298	-5.463	-3.000e-06	0.00987	0.549	1.825
srt_000_02793	Al ₃ NdNi ₆ Sn ₄	14	-4.421	-4.797	0.000e+00	0.00652	0.636	0.538
srt_000_02839	Co ₇ Sn ₈	15	-4.94	-5.228	1.000e-06	0.00577	0.581	0.628
srt_000_02859	Fe ₇ La ₂ Sb ₂ Sn ₃	14	-5.84	-6.173	-1.900e-05	0.00942	0.653	0.691
srt_000_02885	Co ₇ Sn ₈	15	-4.815	-5.136	-5.000e-06	0.00757	0.246	0.879
srt_000_02959	Fe ₇ Na ₈	15	-3.526	-3.983	1.000e-06	0.00612	1.279	1.319
srt_000_02989	Ru ₆ Sn ₁₄	20	-4.58	-5.362	-3.000e-05	0.0053	0.632	1.724
srt_000_03141	Ga ₄ Ni ₆ Sr ₄	14	-3.753	-3.925	0.000e+00	0.00878	0.947	0.976
srt_000_03227	Co ₆ Na ₃ Tl	10	-3.783	-4.268	-3.000e-06	0.00579	0.715	0.838
srt_000_03291	Ba ₂ Ni ₆ Sn ₄	12	-4.373	-4.559	0.000e+00	0.00491	1.283	0.771
srt_000_03316	Ba ₂ Co ₆ SbSn ₄	13	-4.817	-5.043	-2.000e-06	0.0085	0.592	1.01
srt_000_03332	Cs ₂ Ru ₆ Se ₄	12	-5.345	-5.83	-1.400e-05	0.00944	0.678	0.478
srt_000_03334	Fe ₉ Ge ₇ Ho	17	-6.076	-6.422	0.000e+00	0.00575	1.082	1.533
srt_000_03377	Ni ₆ Sn ₈	14	-4.463	-4.626	-1.000e-06	0.00836	0.327	0.263
srt_000_03436	Fe ₆ Se ₆	12	-5.554	-5.983	1.000e-06	0.00554	0.359	0.994
srt_000_03441	Co ₆ Ge ₅ Rb ₂	13	-4.586	-4.992	-3.000e-06	0.00903	1.341	0.793
srt_000_03456	Cs ₈ Yb ₆	14	-0.723	-0.952	-8.200e-05	0.0056	1.555	2.924
srt_000_03468	KLa ₂ Ru ₆ Sb ₅	14	-5.936	-6.415	-5.000e-06	0.00839	1.274	0.877
srt_000_03476	Cs ₂ Tb ₆ Te ₄	12	-3.472	-3.968	-4.000e-06	0.00493	1.894	1.457
srt_000_03496	Cs ₂ PdRu ₆ Se ₅	14	-5.47	-5.724	-2.000e-06	0.00576	0.59	1.549
srt_000_03510	Ce ₃ GeNi ₁₀ Sn ₂	16	-5.382	-5.592	5.000e-06	0.0081	0.914	1.217
srt_000_03588	Cs ₈ Yb ₆	14	-0.812	-0.953	0.000e+00	0.00225	1.204	1.104
srt_000_03603	Ni ₆ Sn ₅ Tl	12	-4.203	-4.536	3.000e-06	0.00587	1.25	0.985
srt_000_03610	LaRu ₇ Sn ₇	15	-5.913	-6.402	4.000e-06	0.00427	0.73	0.604

Table S11. The profile of generated materials with Small rhombitrihexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
srt_000_03702	Na ₂ Ni ₆ Sn ₇	15	-4.026	-4.264	-6.000e-06	0.00772	0.72	1.499
srt_000_03723	CaNdNi ₆ Sn ₆	14	-4.45	-4.707	-3.000e-06	0.00898	0.869	0.602
srt_000_03765	Ge ₂ Ni ₁₀ Pr ₂ Sn ₂	16	-5.126	-5.391	4.000e-06	0.00632	1.091	1.696
srt_000_03768	La ₅ Ni ₆ Sn ₃	14	-5.129	-5.349	2.000e-06	0.00649	0.814	1.261
srt_000_03785	Al ₃ Ge ₃ LiMn ₇ Sb	15	-5.696	-6.074	-9.000e-06	0.0076	0.481	1.385
srt_000_03803	AlBa ₂ Ca ₂ Co ₇ SbSn	14	-4.616	-4.827	4.000e-06	0.00738	0.793	0.742
srt_000_04036	Ga ₅ Nd ₃ Ru ₈	16	-6.203	-6.54	0.000e+00	0.00528	1.152	2.274
srt_000_04051	Co ₇ STe ₆	14	-4.772	-5.165	1.000e-06	0.00937	1.022	1.333
srt_000_04061	Cs ₇ Tb ₆	13	-0.83	-0.953	2.100e-05	0.00582	2.233	2.298
srt_000_04112	GeMn ₆ NdPrSn ₅	14	-5.889	-6.202	-1.700e-05	0.0068	1.142	1.925
srt_000_04269	AgCo ₆ K ₂ S ₈	17	-4.853	-5.141	-4.000e-06	0.00933	0.471	0.62
srt_000_04292	EuGe ₅ Ni ₇	13	-4.796	-5.16	-1.000e-06	0.00948	0.563	1.554
srt_000_04303	Co ₆ PrSnSr ₃ Yb ₃	14	-3.99	-4.228	1.100e-05	0.00752	1.355	1.617
srt_000_04409	Co ₆ PSn ₃ Tl ₂	12	-4.72	-5.092	2.000e-06	0.00965	0.729	0.598
srt_000_04425	Ce ₃ GeNi ₇ Sn ₄	15	-5.179	-5.385	-1.000e-06	0.00881	0.655	1.032
srt_000_04432	CdRbRu ₆ Sn ₂	10	-5.014	-6.121	-1.000e-06	0.00706	0.79	1.575
srt_000_04433	Ge ₄ Ni ₇ Sn ₄	15	-4.663	-4.887	1.000e-06	0.00505	0.62	0.609
srt_000_04444	GaMn ₆ Sn ₈	15	-5.322	-5.618	-6.000e-06	0.00807	0.872	1.17
srt_000_04446	Co ₆ GeLi ₅ SbSr ₂	15	-4.02	-4.197	-1.200e-05	0.0067	0.763	0.69
srt_000_04465	GeMn ₆ Sn ₅ Tl ₄	16	-4.523	-5.057	-5.000e-06	0.00518	0.881	1.373
srt_000_04493	Cs ₈ Tb ₆	14	-1.801	-2.013	-3.000e-05	0.00456	1.388	1.595
srt_000_04519	La ₄ MgNi ₆ Sr ₃	14	-3.891	-4.319	-2.100e-05	0.00981	0.727	0.465
srt_000_04529	AgMn ₆ S ₅ Tl ₂	14	-5.568	-5.933	-1.220e-04	0.00884	0.683	1.154
srt_000_04572	As ₂ Cl ₂ Co ₆ Cs ₂	12	-4.301	-4.846	-5.000e-06	0.00569	2.082	2.849
srt_000_04581	Lu ₃ Mn ₆ Sn ₆	15	-4.96	-5.984	-7.000e-06	0.00943	1.482	2.315
srt_000_04607	Al ₂ Fe ₁₀ Ge ₂ NdScSi ₃	19	-6.411	-6.689	-1.000e-05	0.00661	0.574	1.604
srt_000_04721	Fe ₇ SbSi ₉ Tm	18	-6.026	-6.575	0.000e+00	0.00548	1.232	1.494
srt_000_04727	Co ₆ Sn ₈	14	-4.721	-5.122	0.000e+00	0.00708	0.765	0.647
srt_000_04737	Cs ₈ Nd ₆	14	-1.839	-2.137	7.000e-06	0.00237	1.897	2.417
srt_000_04778	Cs ₄ Sn ₂ Yb ₆	12	-1.393	-1.736	-6.000e-06	0.0042	2.188	2.342
srt_000_04793	Mn ₆ SbSn ₇	14	-5.487	-5.822	-2.000e-06	0.0097	1.183	1.023
srt_000_04847	Ca ₃ Ni ₇ Sn ₃	13	-4.318	-4.499	-1.900e-05	0.00805	0.422	1.621
srt_000_04875	Co ₈ Sm ₂ Sn ₄ Ti ₂	16	-5.991	-6.168	0.000e+00	0.0072	0.479	0.796
srt_000_04893	Co ₆ Sn ₆ Sr ₂	14	-4.692	-4.911	-2.200e-05	0.00885	0.976	0.684
srt_000_04984	EuNi ₈ Sn ₅	14	-4.496	-4.876	-5.000e-06	0.00718	0.514	1.706
srt_000_04988	Co ₉ Ge ₇ Zr ₂	18	-6.026	-6.363	0.000e+00	0.00542	0.546	0.647
srt_000_05005	AsCaLa ₄ Ni ₆ Si ₂	14	-5.097	-5.509	-7.300e-05	0.00827	1.377	1.999
srt_000_05048	Co ₆ CsS ₇ Tl	15	-5.065	-5.369	2.000e-06	0.0082	0.673	0.676
srt_001_00011	AlGeNi ₇ Sm ₅	14	-4.856	-5.27	-3.000e-06	0.00541	0.939	1.433
srt_001_00079	Co ₆ KS _n ₆	13	-4.783	-4.955	-8.000e-06	0.00662	0.559	0.675
srt_001_00089	EuRu ₆ Sr ₇	14	-4.611	-4.709	-3.200e-05	0.00533	0.82	1.628
srt_001_00090	Cs ₈ Nd ₆	14	-1.79	-2.139	-4.000e-06	0.00783	1.516	2.772
srt_001_00097	Ni ₇ Sn ₈	15	-4.505	-4.679	-6.000e-06	0.00881	0.608	1.969
srt_001_00099	Ga ₆ Ni ₆ Sr ₂	14	-3.941	-4.136	-6.000e-06	0.00869	0.673	1.669
srt_001_00127	BaCa ₄ Fe ₆ NdSi ₂	14	-4.973	-5.219	-3.000e-06	0.00737	0.79	1.649
srt_001_00161	Co ₆ Ga ₃ Sn ₅	14	-4.83	-4.952	-4.000e-06	0.00612	0.225	0.684
srt_001_00181	Al ₇ DyFe ₆	14	-5.405	-5.776	8.000e-06	0.0048	0.847	0.622
srt_001_00186	La ₂ Ni ₁₀ Sn ₃	15	-4.973	-5.322	-1.400e-05	0.00884	1.033	2.114
srt_001_00217	Ni ₆ Sn ₃ Sr ₂ Y ₂ Zn	14	-4.611	-4.722	-1.000e-06	0.00805	0.558	0.418
srt_001_00302	Co ₈ Ge ₇ Sr ₂	17	-5.243	-5.444	-1.900e-05	0.00916	0.723	1.176
srt_001_00336	Ca ₅ CeGa ₂ Ni ₆	14	-3.891	-4.072	-8.000e-06	0.00714	0.628	3.017

Table S11. The profile of generated materials with Small rhombitrihexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
srt_001_00371	Ru ₆ Sn ₉	15	-5.322	-5.824	-5.000e-06	0.00468	0.352	0.926
srt_001_00397	Ba ₂ Ge ₅ Ni ₆	13	-4.606	-4.774	-2.000e-06	0.00983	0.436	1.058
srt_001_00484	Ba ₄ Co ₆ Sn ₄	14	-4.458	-4.726	-2.000e-06	0.00759	1.174	0.916
srt_001_00499	Ba ₄ Co ₆ Sn ₄	14	-4.498	-4.756	2.800e-05	0.00982	1.55	1.883
srt_001_00514	Al ₂ Ce ₆ Co ₇	15	-6.145	-6.342	-6.000e-06	0.0085	0.466	0.587
srt_001_00526	AlGeRu ₆ Te ₅	13	-5.429	-6.033	-7.000e-06	0.00545	1.737	2.327
srt_001_00542	Ge ₈ Mn ₆ NdZr ₃	18	-6.091	-6.835	0.000e+00	0.00733	0.464	0.692
srt_001_00577	Eu ₂ Ru ₆ Sn ₇	15	-5.281	-5.758	-3.000e-06	0.00646	0.817	0.853
srt_001_00590	Ni ₆ SbSn ₇	14	-4.507	-4.657	2.000e-06	0.0076	0.353	0.34
srt_001_00633	Cs ₈ Yb ₆	14	-0.766	-0.95	-2.000e-06	0.00274	1.191	1.688
srt_001_00644	La ₂ Ni ₆ Sn ₅ Y	14	-5.207	-5.295	-5.000e-06	0.00734	0.419	0.391
srt_001_00805	Ce ₅ Ge ₄ Ru ₆	15	-6.847	-7.238	0.000e+00	0.00585	1.126	0.922
srt_001_00829	CdMgRu ₆ Sn ₁₀	18	-4.56	-5.312	-1.200e-05	0.00462	1.567	1.738
srt_001_00893	Co ₈ Ge ₄ NdSn	14	-5.558	-5.926	-1.000e-06	0.004	0.749	0.753
srt_001_00937	Al ₃ Ba ₃ GdNi ₆ Sn	14	-4.273	-4.44	-3.000e-06	0.00975	0.93	0.872
srt_001_00990	Co ₇ Na ₄	11	-4.041	-4.428	-1.100e-05	0.0064	1.37	0.993
srt_001_01124	Cd ₂ Ge ₃ Ni ₆ Sn ₂	13	-4.004	-4.192	-1.000e-06	0.00641	0.694	0.623
srt_001_01125	Co ₆ Ge ₂ Sn ₆	14	-5.134	-5.259	-1.000e-06	0.00854	0.931	0.63
srt_001_01131	Mn ₈ SbSn ₁₀ Y	20	-5.536	-5.885	-4.000e-05	0.00655	0.545	1.406
srt_001_01139	Fe ₆ Rb ₂ Te ₇	15	-4.49	-4.812	-5.000e-06	0.00663	1.218	1.285
srt_001_01160	Ga ₄ Rb ₂ Ru ₇	13	-5.422	-5.656	-5.000e-06	0.00666	0.572	2.901
srt_001_01207	Al ₃ La ₄ Ni ₆	13	-5.036	-5.227	-4.300e-05	0.00732	0.985	1.541
srt_001_01211	Ni ₆ Sn ₇ Tm	14	-4.56	-4.776	1.000e-06	0.00842	0.278	0.454
srt_001_01253	Fe ₆ GaMnNa ₂ Sn ₄	14	-4.777	-5.385	-1.000e-05	0.00873	1.391	1.737
srt_001_01255	Co ₆ Ga ₄ SiSr ₂	13	-4.431	-4.853	-3.800e-05	0.00924	1.008	3.887
srt_001_01256	Mn ₆ Sn ₆ Sr ₂	14	-5.226	-5.657	1.800e-05	0.00662	1.042	2.382
srt_001_01327	PdRu ₆ Sn ₆ TiY	15	-5.631	-6.561	0.000e+00	0.00436	1.036	1.162
srt_001_01374	Cs ₇ Yb ₈	15	-0.75	-1.005	-9.400e-05	0.00582	1.203	1.546
srt_001_01377	Cs ₇ Yb ₆	13	-0.745	-0.954	-3.000e-06	0.00155	2.234	3.947
srt_001_01398	GeNi ₆ Sn ₇	14	-4.591	-4.683	-1.000e-06	0.00729	0.481	0.275
srt_001_01450	Co ₆ SSn ₆ Zr	14	-5.501	-5.622	-1.000e-06	0.00651	0.516	0.671
srt_001_01479	Ba ₄ Mn ₆ Sn ₄	14	-5.195	-5.404	3.900e-05	0.00553	1.052	0.817
srt_001_01577	Ca ₈ Fe ₇	15	-4.191	-4.565	1.200e-05	0.00815	0.371	0.743
srt_001_01639	Co ₆ Ga ₄ Pr ₂	12	-5.165	-5.516	-1.400e-05	0.00892	1.259	1.341
srt_001_01712	Cs ₇ Yb ₆	13	-0.829	-0.954	-3.000e-06	0.0045	1.711	5.135
srt_001_01886	Co ₁₄ Nd ₂ Sb	17	-6.179	-6.415	-4.000e-05	0.00703	0.568	0.889
srt_001_01901	Co ₈ Ge ₄ LaTe ₃	16	-5.377	-5.645	3.000e-06	0.00575	0.765	0.82
srt_001_01916	Ni ₆ Sn ₃ Sr ₅	14	-3.902	-3.987	-6.000e-06	0.00441	0.661	0.603
srt_001_01931	AlCo ₈ GePr ₄	14	-5.461	-6.009	-1.000e-06	0.00837	1.014	1.66
srt_001_01934	Ni ₆ Sn ₇ Yb	14	-4.348	-4.573	1.000e-06	0.00744	0.338	0.388
srt_001_01936	Ba ₂ Ca ₂ Ni ₆ Sn ₄	14	-4.126	-4.288	-4.000e-06	0.00399	0.654	0.551
srt_001_01958	Cs ₇ Yb ₈	15	-0.703	-0.995	4.000e-06	0.00385	1.787	3.527
srt_001_01992	CoEu ₄ Fe ₆ Sn ₄	15	-4.949	-5.396	-4.000e-06	0.00652	0.778	0.751
srt_001_01993	AlAs ₂ Nd ₃ Ni ₇ Tl	14	-4.934	-5.239	-4.000e-06	0.00891	1.35	1.573
srt_001_02051	Cs ₂ Ru ₆ Sn ₂ Te ₃	13	-5.309	-5.598	-2.000e-06	0.00604	0.687	0.608
srt_001_02101	Ba ₂ Ru ₇ Sn ₃ Sr	13	-5.719	-6.155	-2.000e-06	0.00588	0.842	1.938
srt_001_02116	Cs ₈ Yb ₆	14	-0.855	-0.952	-5.000e-06	0.00328	1.631	1.832
srt_001_02121	Ga ₂ Mn ₉ Sb ₈	19	-5.815	-6.033	0.000e+00	0.00584	0.542	1.219
srt_001_02142	BaMn ₆ Se ₇	14	-5.863	-6.202	-3.700e-05	0.005	0.348	0.948
srt_001_02147	Dy ₆ Rb ₈	14	-1.827	-2.063	-1.600e-05	0.00536	1.553	2.328
srt_001_02191	Co ₆ Sn ₈	14	-4.671	-5.121	-3.000e-06	0.0073	0.794	1.146

Table S11. The profile of generated materials with Small rhombitrihexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
srt_001_02265	Ba ₄ Ni ₆ Sn ₄	14	-4.085	-4.265	-2.000e-06	0.00586	0.722	1.213
srt_001_02278	K ₂ Ru ₆ Se ₂ Sn ₂ Te ₂	14	-5.456	-5.651	-2.000e-06	0.00737	0.393	0.393
srt_001_02315	Ce ₆ Ni ₉	15	-5.699	-5.883	-2.000e-06	0.00723	0.674	1.376
srt_001_02337	Co ₇ Ge ₉	16	-5.312	-5.595	-1.100e-05	0.00652	0.998	1.71
srt_001_02349	GeRu ₆ Sn ₇ Tb	15	-5.47	-6.012	-2.000e-06	0.00497	0.743	1.219
srt_001_02410	Ni ₆ Sn ₇	13	-4.291	-4.63	-2.000e-06	0.00727	0.799	1.318
srt_001_02413	As ₂ Mn ₆ Sb ₆	14	-5.715	-6.216	0.000e+00	0.00724	0.813	0.952
srt_001_02418	La ₄ MgNi ₆ Si ₃	14	-5.333	-5.475	2.000e-06	0.00658	0.851	1.572
srt_001_02450	Al ₂ Co ₉ Sr ₆	17	-4.337	-4.425	1.000e-05	0.00987	0.302	1.197
srt_001_02462	Co ₆ Er ₂ Nd ₃ Sn ₃	14	-5.609	-5.692	2.000e-06	0.00716	0.742	0.704
srt_001_02508	Cs ₈ Nd ₆	14	-1.822	-2.134	-2.000e-06	0.00351	1.728	1.514
srt_001_02572	BrGa ₅ Ru ₆ Sn ₂	14	-4.949	-5.416	-2.000e-06	0.00756	0.809	2.454
srt_001_02612	Ba ₂ Co ₈ Sn ₆	16	-4.893	-5.166	-2.000e-06	0.00686	0.401	0.748
srt_001_02656	Ag ₂ Cd ₂ RbRu ₆ Sb ₆	17	-4.504	-5.039	-2.000e-06	0.00744	1.636	2.629
srt_001_02668	Mn ₆ Sn ₈	14	-5.481	-5.771	0.000e+00	0.00891	0.888	1.045
srt_001_02679	Cs ₇ Yb ₆	13	-0.843	-0.953	-1.000e-06	0.00102	2.267	4.065
srt_001_02726	Al ₁₀ Ru ₉ Ti	20	-6.383	-6.81	0.000e+00	0.00696	1.157	1.187
srt_001_02788	Al ₆ Co ₆ SnY ₂	15	-5.373	-5.662	-1.100e-05	0.00804	1.116	1.594
srt_001_02802	Ge ₃ Mn ₆ Sn ₅ Tl	15	-5.168	-5.639	1.000e-06	0.00389	1.009	3.705
srt_001_02807	Co ₆ Te ₆	12	-4.582	-5.083	-2.000e-05	0.00799	1.576	1.205
srt_001_02851	Cs ₈ Dy ₆	14	-1.66	-1.994	-2.500e-05	0.00978	1.858	2.142
srt_001_02853	Cs ₈ Dy ₆	14	-1.837	-1.996	2.000e-06	0.00307	1.164	1.152
srt_001_02876	Ni ₆ Sn ₆ Y ₂	14	-4.938	-5.23	1.000e-06	0.00776	0.608	0.524
srt_001_02934	Co ₆ Ge ₇ Y	14	-5.632	-5.794	3.000e-06	0.00963	0.63	0.718
srt_001_02944	Cs ₈ Tb ₆	14	-1.853	-2.014	2.000e-06	0.00271	1.088	1.245
srt_001_02959	Cs ₆ PbYb ₆	13	-1.022	-1.22	8.000e-06	0.00363	1.004	1.374
srt_001_03036	Cs ₈ Dy ₆	14	-1.812	-1.993	-1.000e-05	0.00497	1.148	1.468
srt_001_03058	Mn ₁₀ ScSn ₈	19	-5.997	-6.38	-2.000e-05	0.00985	0.694	0.765
srt_001_03060	Bi ₇ Co ₇ Er	15	-5.147	-5.208	1.200e-05	0.00793	0.145	0.262
srt_001_03086	Ba ₃ Co ₆ Ga ₂ GeTe	13	-4.473	-4.795	1.000e-06	0.00704	0.401	1.894
srt_001_03155	Co ₆ Sn ₇	13	-4.787	-5.097	-1.000e-06	0.00858	0.869	0.478
srt_001_03179	Cs ₇ Yb ₆	13	-0.739	-0.951	-4.000e-06	0.00203	1.182	1.986
srt_001_03203	BaLu ₄ PrRu ₆ Sn	13	-6.077	-6.431	-1.400e-05	0.00862	0.682	1.896
srt_001_03205	AlCo ₉ Nd ₃ Pr ₂ Si	16	-5.737	-6.051	-3.000e-06	0.00702	1.038	1.4
srt_001_03281	CaEu ₂ MgNi ₉ SnSr	15	-4.028	-4.274	-2.000e-06	0.0078	1.124	0.814
srt_001_03301	Ru ₇ Sn ₉	16	-5.646	-6.04	1.000e-06	0.00624	1.125	1.561
srt_001_03313	Ni ₆ Sn ₈	14	-4.387	-4.632	-3.000e-06	0.00459	0.644	0.509
srt_001_03316	AuBiCo ₆ EuSe ₆	15	-4.639	-4.987	-5.000e-06	0.00945	0.758	1.945
srt_001_03328	Fe ₈ Sn ₈	16	-5.169	-5.735	-1.000e-06	0.00641	1.005	1.232
srt_001_03335	Ge ₅ Mn ₉ Ti ₄	18	-7.279	-7.61	-2.000e-05	0.00744	0.558	0.558
srt_001_03398	Br ₆ Co ₆	12	-3.689	-4.17	-3.000e-06	0.00625	1.208	2.161
srt_001_03465	Co ₈ Ge ₈ Li	17	-5.265	-5.602	1.000e-06	0.00818	0.667	1.327
srt_001_03467	La ₂ Ru ₆ Sn ₁₀	18	-5.767	-5.891	-1.000e-05	0.00871	0.404	1.955
srt_001_03468	Co ₈ GeSb ₄ Sr ₃	16	-4.914	-5.181	8.000e-06	0.00792	0.836	1.009
srt_001_03503	Al ₄ Co ₆ Sn ₂ Y	13	-5.196	-5.519	-8.000e-06	0.00708	0.717	0.634
srt_001_03653	Cs ₈ Tb ₆	14	-1.763	-2.014	-2.300e-05	0.00628	1.55	2.137
srt_001_03723	Ba ₂ Ni ₆ Sn ₇	15	-4.46	-4.527	-3.300e-05	0.00855	0.23	0.229
srt_001_03758	Ca ₂ Co ₇ Ge ₆	15	-5.22	-5.437	4.000e-06	0.007	0.706	0.567
srt_001_03773	Ni ₆ Sn ₇	13	-4.469	-4.585	-1.000e-05	0.00875	0.055	0.219
srt_001_03831	Ba ₂ Ru ₆ Sn ₆	14	-5.494	-5.867	1.000e-06	0.00636	0.846	0.613
srt_001_03881	Co ₁₀ Sb ₅ Sn ₄	19	-5.191	-5.453	0.000e+00	0.00769	0.786	2.035

Table S11. The profile of generated materials with Small rhombitrihexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
srt_001_03938	GeMn ₇ Sn ₇ U ₃	18	-6.368	-6.977	0.000e+00	0.00566	1.197	1.263
srt_001_03988	Ni ₆ Sn ₃ Sr ₂ Tl ₃	14	-3.873	-4.025	1.000e-06	0.00455	1.102	0.795
srt_001_03993	Ba ₅ Ge ₃ Ni ₆	14	-3.953	-4.178	-6.000e-06	0.00434	0.716	0.486
srt_001_04025	As ₂ Ge ₂ K ₄ Mn ₆	14	-4.998	-5.317	-1.000e-06	0.00782	0.889	1.059
srt_001_04053	Ru ₇ Sn ₈	15	-5.911	-6.21	-1.000e-06	0.00547	0.685	0.571
srt_001_04070	Ga ₈ Ni ₆	14	-4.069	-4.159	2.000e-06	0.00402	0.358	0.206
srt_001_04118	AgCo ₆ PdSn ₆	14	-4.809	-5.1	-8.000e-06	0.00624	0.778	0.78
srt_001_04201	Co ₇ LaSn ₇	15	-5.035	-5.354	4.000e-06	0.00665	0.802	3.247
srt_001_04208	Ru ₆ Sn ₈	14	-5.558	-6.046	-1.700e-05	0.00592	0.841	0.551
srt_001_04214	Cs ₂ Ru ₆ Se ₄	12	-5.541	-5.83	-1.500e-05	0.00576	0.56	1.048
srt_001_04232	Al ₂ Ge ₂ NdNi ₁₂	17	-5.128	-5.281	-6.000e-06	0.00579	0.439	1.191
srt_001_04244	Co ₆ I ₈ Se	15	-3.382	-3.693	-4.000e-06	0.00978	0.535	1.299
srt_001_04283	Ce ₂ Co ₈ Ga ₃ Ge	14	-5.549	-5.951	-6.000e-06	0.00922	1.018	1.494
srt_001_04285	BrCl ₆ GeRu ₆	14	-4.43	-5.128	-1.000e-05	0.00692	1.222	2.993
srt_001_04305	KNi ₆ Sn ₇	14	-4.347	-4.492	-7.000e-06	0.00822	0.815	1.64
srt_001_04327	MnRu ₈ SbSn ₁₀	20	-5.501	-6.052	-4.000e-05	0.00962	0.615	0.84
srt_001_04346	Ni ₆ Sn ₅ Tm ₃	14	-4.965	-5.072	-4.400e-05	0.00889	0.405	0.256
srt_001_04360	K ₂ Ru ₆ Sb ₂ Sn ₃	13	-5.599	-5.759	0.000e+00	0.00815	0.451	0.439
srt_001_04377	Co ₇ SmSn ₆	14	-5.332	-5.424	1.000e-06	0.0078	0.47	0.503
srt_001_04387	Ce ₂ Fe ₆ Ga ₅	13	-5.471	-5.962	0.000e+00	0.00852	1.109	1.224
srt_001_04443	Ba ₂ Co ₆ Se ₅	13	-4.931	-5.252	-6.200e-05	0.00581	0.712	2.056
srt_001_04444	Co ₆ Ga ₆ KSr	14	-4.236	-4.489	2.000e-06	0.00738	1.174	1.796
srt_001_04502	Mn ₆ Sn ₈	14	-5.597	-5.803	-6.000e-06	0.00746	0.12	0.36
srt_001_04550	CaMn ₆ S ₈	15	-6.147	-6.636	3.000e-06	0.00692	1.334	0.759
srt_001_04557	Ba ₂ Ni ₆ Sn ₅	13	-4.345	-4.488	-9.000e-06	0.00359	0.657	1.222
srt_001_04650	Co ₆ K ₄ Sb ₂ Se ₂	14	-4.367	-4.478	-1.000e-06	0.00629	0.514	0.499
srt_001_04675	Ga ₆ PdRu ₆ U	14	-6.058	-6.51	0.000e+00	0.00546	0.491	1.155
srt_001_04754	Cs ₉ Tb ₆	15	-1.624	-1.926	-8.000e-06	0.00541	1.963	2.579
srt_001_04812	Ga ₄ Ni ₇ Sr ₂	13	-4.161	-4.325	-5.000e-06	0.00752	0.971	0.755
srt_001_04845	BaCo ₆ S ₂ Sn ₂ Sr ₂	13	-4.631	-5.098	4.000e-06	0.00755	1.176	1.422
srt_001_04856	Ce ₈ Co ₆	14	-6.31	-6.561	6.000e-06	0.00764	0.799	1.226
srt_001_04866	Eu ₂ Ni ₆ SnTe ₄ Zn	14	-3.943	-4.247	-6.000e-06	0.00846	0.993	1.294
srt_001_04996	BrCeCo ₇ MgNa ₂ Si ₂ Zn	15	-4.586	-4.884	-2.000e-06	0.00866	1.35	1.944
srt_002_00064	Mn ₇ Se ₇	14	-5.973	-6.352	-2.000e-06	0.00973	0.358	0.944
srt_002_00132	Lu ₈ Ru ₆	14	-6.652	-6.733	-6.000e-06	0.00743	0.633	0.609
srt_002_00142	Cs ₈ Tb ₆	14	-1.697	-2.021	-7.300e-05	0.00891	1.779	2.833
srt_002_00255	BaFe ₆ Ga ₄ GdSr ₂	14	-4.798	-5.088	-6.500e-05	0.00892	1.299	0.951
srt_002_00310	As ₈ Fe ₆	14	-6.086	-6.204	-5.000e-06	0.00444	0.658	0.644
srt_002_00335	CaEuGe ₂ Ni ₈ Se ₈	20	-4.368	-4.687	-1.100e-05	0.0073	0.923	2.244
srt_002_00386	Mn ₆ S ₄ Tl ₄	14	-5.378	-5.686	1.000e-06	0.00549	0.583	0.356
srt_002_00531	Br ₅ Mn ₇ P ₂	14	-5.134	-5.892	0.000e+00	0.00736	1.255	1.043
srt_002_00558	CaNi ₆ Sn ₆	13	-4.169	-4.626	-2.000e-05	0.00964	0.795	2.695
srt_002_00570	Er ₂ Fe ₇ Sn ₅	14	-5.405	-6.065	1.000e-06	0.00973	1.499	1.34
srt_002_00586	Cs ₈ Nd ₆	14	-1.812	-2.139	1.300e-05	0.0036	1.701	3.441
srt_002_00589	Bi ₄ Ge ₃ Ni ₇ Sn	15	-4.575	-4.801	0.000e+00	0.00462	0.737	0.531
srt_002_00703	Co ₆ Ge ₈	14	-5.347	-5.578	5.000e-06	0.00875	0.785	1.146
srt_002_00729	Ni ₆ Sn ₈	14	-4.52	-4.633	-7.000e-06	0.00909	0.52	0.616
srt_002_00760	Mn ₆ Sr ₈	14	-3.761	-4.299	0.000e+00	0.00714	0.999	2.552
srt_002_00763	CeGeNi ₁₀ Sm	13	-5.315	-5.524	3.000e-06	0.00744	0.648	0.442
srt_002_00777	Ni ₆ Sn ₈	14	-4.519	-4.628	-2.000e-06	0.00631	0.375	0.355
srt_002_00798	Ni ₆ Sn ₈	14	-4.247	-4.651	-3.000e-06	0.00536	1.224	1.391

Table S11. The profile of generated materials with Small rhombitrihexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
srt_002_00816	AlBiGe ₄ NdRu ₆ SbSn	15	-5.733	-6.287	0.000e+00	0.00646	0.441	1.337
srt_002_00862	Co ₆ La ₈	14	-5.795	-5.898	-4.000e-06	0.00752	0.358	3.447
srt_002_00921	Ba ₂ Co ₆ Sn ₄	12	-4.833	-5.16	-1.200e-05	0.0057	1.552	0.939
srt_002_00934	Co ₆ La ₂ Sn ₆	14	-5.301	-5.446	-2.000e-06	0.00666	0.355	0.302
srt_002_00998	Mn ₆ Nd ₂ Sn ₇	15	-5.037	-6.029	-4.000e-06	0.00586	0.874	1.42
srt_002_01007	Cs ₈ Yb ₆	14	-0.846	-0.954	-2.000e-06	0.0022	1.636	2.284
srt_002_01029	Ni ₇ Sn ₈	15	-4.435	-4.683	-2.000e-06	0.00774	0.603	2.13
srt_002_01148	As ₂ CaGeKMgNd ₂ Ni ₇ Sb ₂ Ir	18	-4.396	-4.556	0.000e+00	0.00771	1.034	2.341
srt_002_01152	Co ₇ Sn ₈	15	-4.886	-5.203	-1.000e-06	0.00489	1.209	1.524
srt_002_01162	Ru ₇ Sn ₆ Y ₅	18	-6.371	-6.839	0.000e+00	0.00734	0.936	2.788
srt_002_01188	Ru ₆ Sn ₈	14	-5.513	-6.067	-1.100e-05	0.00658	1.395	0.919
srt_002_01210	Cs ₈ Dy ₆	14	-1.793	-1.994	-5.000e-06	0.00872	1.354	2.183
srt_002_01229	AlNa ₂ Ni ₉	12	-4.163	-4.471	1.200e-05	0.00688	0.593	1.196
srt_002_01255	Co ₆ Sn ₈	14	-5.078	-5.13	-1.800e-05	0.00482	0.251	0.241
srt_002_01277	AsGeNi ₇ Sn ₃	13	-4.602	-4.847	0.000e+00	0.00671	0.429	0.468
srt_002_01283	Fe ₈ Ge ₂ PrSi ₅ Tm	17	-6.173	-6.659	-1.000e-05	0.00668	1.359	2.489
srt_002_01301	Cs ₇ Yb ₆	13	-0.782	-0.952	1.000e-06	0.00212	2.274	2.127
srt_002_01360	BaGa ₄ La ₃ Ni ₆	14	-4.568	-4.718	-2.100e-05	0.00935	0.61	0.36
srt_002_01387	Ni ₈ Sn ₈	16	-4.605	-4.747	-6.000e-06	0.00643	0.559	0.621
srt_002_01389	Ni ₆ Sn ₇	13	-4.504	-4.59	0.000e+00	0.00902	0.437	0.237
srt_002_01393	Cs ₂ Dy ₆ Rb ₆	14	-1.854	-2.05	-1.200e-05	0.00252	1.276	1.364
srt_002_01440	LaNi ₁₁ Sr	13	-4.879	-5.144	7.000e-06	0.00669	0.445	0.547
srt_002_01476	Ga ₉ Ni ₆ Sr	16	-3.731	-3.992	5.000e-06	0.00287	0.688	2.467
srt_002_01559	Mn ₆ Sn ₈	14	-5.47	-5.805	2.000e-06	0.00456	0.749	0.665
srt_002_01662	Mn ₆ Sn ₈	14	-5.556	-5.806	0.000e+00	0.00665	0.082	0.459
srt_002_01673	Co ₆ GeNd ₃ SmSn ₃	14	-5.616	-5.769	-2.800e-05	0.00832	0.546	0.367
srt_002_01696	CeNi ₉ PrSn ₅	16	-5.169	-5.195	-4.000e-06	0.0073	0.557	0.612
srt_002_01716	Ca ₂ Ru ₆ Sn ₆ Y	15	-5.849	-6.0	-2.000e-06	0.00603	0.797	0.602
srt_002_01739	Ga ₄ Nd ₄ Ni ₈	16	-4.724	-5.004	0.000e+00	0.00866	0.927	2.183
srt_002_01807	Co ₆ Se ₆ Zr ₃	15	-5.833	-6.366	-2.000e-06	0.00624	1.301	1.587
srt_002_01822	As ₄ Ru ₆ Sr ₄	14	-5.834	-6.01	-3.800e-05	0.00689	0.749	0.525
srt_002_01922	Co ₆ Pd ₃ Sn ₆	15	-4.75	-5.544	-4.000e-06	0.00562	0.402	1.125
srt_002_01969	Ga ₄ Ni ₈ Sb ₂ Y ₂	15	-4.94	-5.166	-1.500e-05	0.00676	0.531	0.638
srt_002_01974	Co ₁₁ Ge ₅ Y ₂	18	-6.119	-6.378	-1.000e-05	0.006	0.838	0.908
srt_002_02009	GeK ₄ Ni ₇ Sn ₃	15	-3.872	-4.018	-4.000e-06	0.00982	0.699	0.683
srt_002_02015	Cs ₈ Tb ₆	14	-1.746	-2.015	-1.800e-05	0.00309	1.709	2.826
srt_002_02098	Ru ₉ Sn ₅ Sr ₂	16	-6.074	-6.479	0.000e+00	0.00594	0.772	1.385
srt_002_02121	Cs ₉ Dy ₆	15	-1.582	-1.907	-4.400e-05	0.00474	1.854	4.224
srt_002_02206	AlBRu ₉ Sn ₅ TiU	18	-6.869	-7.352	-1.000e-05	0.00961	0.377	0.636
srt_002_02245	Co ₆ GaLaMg ₄ NdY	14	-4.481	-4.845	1.000e-06	0.00429	1.033	0.85
srt_002_02325	Co ₆ PrSn ₇	14	-5.079	-5.266	0.000e+00	0.00755	0.762	1.268
srt_002_02354	Cs ₂ Ru ₇ Sn ₄	13	-5.507	-5.948	-5.000e-06	0.00841	1.064	0.672
srt_002_02364	Co ₇ Sn ₈	15	-4.821	-5.218	-2.400e-05	0.00945	0.526	0.949
srt_002_02394	BaCo ₆ GeSn ₅	13	-4.762	-5.147	1.000e-06	0.00785	0.795	0.954
srt_002_02513	Cs ₈ Yb ₆	14	-0.745	-0.951	-1.000e-06	0.00277	1.039	1.248
srt_002_02523	Cs ₈ Tb ₆	14	-1.729	-2.015	-5.000e-06	0.0059	1.623	1.321
srt_002_02567	Ni ₁₅ Sn ₅	20	-4.882	-5.135	0.000e+00	0.00549	0.431	1.67
srt_002_02673	K ₃ Ni ₇ Si ₄	14	-4.24	-4.542	-2.900e-05	0.00738	0.93	0.979
srt_002_02678	Ba ₄ Ga ₅ Ni ₆ Sn	16	-3.77	-3.929	0.000e+00	0.0062	0.778	1.612
srt_002_02737	As ₃ Cs ₄ Mn ₆ S	14	-5.101	-5.388	-9.000e-06	0.00583	1.848	1.644
srt_002_02761	Co ₇ Ga ₂ Nd ₂ PrSn ₃	15	-5.185	-5.548	-1.000e-06	0.00476	0.817	0.694

Table S11. The profile of generated materials with Small rhombitrihexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
srt_002_02763	Cs ₂ Ru ₇ Sn ₃	12	-5.793	-6.094	-1.000e-06	0.00279	1.027	1.477
srt_002_02773	CeNi ₆ Sn ₆	13	-4.488	-4.887	-3.600e-05	0.00923	0.711	0.843
srt_002_02797	Fe ₆ Ga ₃ GeLu ₄ Si	15	-5.462	-5.85	-1.000e-06	0.00593	0.864	1.545
srt_002_02813	Cs ₆ Tb ₆	12	-1.82	-2.291	-9.000e-06	0.00367	4.524	3.475
srt_002_02881	AgGaMn ₆ Sn ₇	15	-4.917	-5.443	-1.000e-06	0.00734	0.903	0.794
srt_002_02922	Ru ₆ Sn ₇	13	-5.563	-6.067	-3.000e-06	0.00587	0.737	0.754
srt_002_02932	Ge ₂ Mn ₆ Sn ₇	15	-5.228	-5.753	0.000e+00	0.00458	1.042	1.823
srt_002_02947	Co ₆ Gd ₂ Sn ₆	14	-5.309	-5.448	0.000e+00	0.00623	0.415	0.335
srt_002_02949	Ni ₆ Sn ₆	12	-4.409	-4.558	0.000e+00	0.00663	0.622	0.475
srt_002_02980	Ca ₄ Mn ₆ Sn ₃ Tb	14	-5.025	-5.495	-6.000e-06	0.00706	0.988	0.694
srt_002_02993	Cs ₈ Yb ₆	14	-0.738	-0.95	0.000e+00	0.00269	1.771	2.004
srt_002_03076	Mg ₈ Ni ₇	15	-3.235	-3.449	0.000e+00	0.00822	0.63	0.598
srt_002_03115	CaCo ₈ Ge ₄ Y ₃	16	-5.874	-6.191	3.000e-06	0.00746	1.607	4.026
srt_002_03155	GeMn ₆ P ₇	14	-6.375	-7.093	-1.400e-05	0.00635	1.134	1.931
srt_002_03163	Co ₆ Se ₈ Sn	15	-4.91	-5.161	-3.000e-06	0.00775	0.702	1.224
srt_002_03196	Ba ₂ NdRu ₇ Sb ₂ Sn ₆	18	-5.63	-5.815	-1.000e-05	0.00582	0.777	1.0
srt_002_03240	Ba ₂ Ru ₆ Sn ₆	14	-5.427	-5.861	0.000e+00	0.00869	0.588	0.598
srt_002_03353	Ni ₇ Sn ₉	16	-4.428	-4.603	-1.000e-06	0.00885	0.875	0.855
srt_002_03375	As ₄ Mn ₇ Tl ₂	13	-5.881	-6.351	-2.000e-06	0.00746	0.804	0.424
srt_002_03379	Ru ₇ Se ₂ Sn ₄ Sr	14	-5.877	-6.356	-4.000e-06	0.00717	0.939	1.42
srt_002_03425	CoLa ₄ Ru ₁₀ Si ₄ Tc	20	-7.314	-7.699	-6.000e-05	0.00583	0.871	3.325
srt_002_03459	Ni ₆ Sn ₇	13	-4.262	-4.585	-1.000e-06	0.00919	0.595	0.565
srt_002_03483	Co ₆ Ge ₃ NdTl ₅	15	-4.355	-4.662	-1.400e-05	0.009	0.337	1.075
srt_002_03511	Cs ₆ Yb ₆	12	-0.727	-0.943	-1.900e-05	0.00335	1.176	1.197
srt_002_03558	Ca ₂ Co ₆ Sn ₆	14	-4.871	-4.946	-2.100e-05	0.00421	0.487	0.397
srt_002_03579	AlGeNi ₆ SbSn ₅	14	-4.65	-4.698	0.000e+00	0.00815	0.109	0.161
srt_002_03609	Eu ₂ Ga ₃ Ge ₇ Ni ₆	18	-4.298	-4.56	-2.000e-06	0.00531	0.933	2.411
srt_002_03625	I ₆ Mn ₆ Sn ₃	15	-4.235	-4.716	4.000e-06	0.00957	0.409	0.857
srt_002_03651	Cs ₈ Yb ₆	14	-0.851	-0.954	-6.000e-06	0.00481	1.489	2.261
srt_002_03663	CeCo ₆ Sn ₈	15	-5.084	-5.236	2.000e-06	0.00874	0.801	1.362
srt_002_03703	Ba ₂ Co ₆ Sn ₄	12	-4.755	-5.131	0.000e+00	0.0062	1.553	2.786
srt_002_03724	Cs ₅ RbYb ₇	13	-0.762	-1.0	0.000e+00	0.00259	1.078	3.057
srt_002_03757	Cs ₈ Nd ₆	14	-1.949	-2.136	-2.000e-06	0.00283	1.27	2.232
srt_002_03761	AlNi ₇ Sn ₅ Sr	14	-4.462	-4.648	-4.000e-06	0.00675	0.656	0.944
srt_002_03850	GdRu ₁₂ Si ₂ Sn ₃ Y ₂	20	-7.211	-7.657	0.000e+00	0.0047	0.716	1.139
srt_002_03874	Al ₇ Mn ₆ Sr ₂	15	-5.072	-5.526	0.000e+00	0.00628	1.373	1.042
srt_002_03912	CaFe ₆ La ₂ Sn ₄	13	-5.458	-5.844	-2.000e-06	0.00723	0.882	1.546
srt_002_03953	Al ₅ Co ₆ Tl ₂	13	-4.719	-4.863	8.000e-06	0.00966	0.534	2.293
srt_002_04033	AlGa ₄ GdNi ₆ Pr	13	-4.506	-4.769	0.000e+00	0.00356	1.006	1.259
srt_002_04034	BrKRu ₆ S ₅ Sn ₂	15	-5.745	-6.041	-2.000e-06	0.00738	0.664	1.18
srt_002_04063	Mg ₈ Ni ₇	15	-3.348	-3.451	-1.300e-05	0.00887	0.623	1.377
srt_002_04073	Cs ₇ Yb ₇	14	-0.815	-0.976	-1.300e-05	0.00312	2.163	3.336
srt_002_04099	Bi ₂ Eu ₂ Ni ₆ Sn ₄	14	-4.282	-4.589	-3.000e-06	0.00803	1.157	1.268
srt_002_04175	Ba ₂ Ge ₈ Ru ₆	16	-5.708	-6.009	0.000e+00	0.00565	0.555	0.577
srt_002_04186	Cs ₄ SbYb ₆	11	-1.084	-1.458	-2.600e-05	0.00317	2.965	2.157
srt_002_04286	AsCl ₄ Mn ₆ SSb	13	-5.277	-5.765	-1.000e-06	0.00831	0.928	1.238
srt_002_04323	Co ₆ Sn ₈	14	-4.842	-5.128	-2.800e-05	0.00765	0.667	0.856
srt_002_04367	GaNi ₆ Sn ₂ Tl ₅	14	-3.702	-3.808	-2.000e-06	0.00433	0.348	0.526
srt_002_04375	Ge ₇ Nd ₃ Ru ₇	17	-6.194	-6.754	0.000e+00	0.00644	1.27	1.449
srt_002_04407	Ge ₉ LaPrRu ₆	17	-5.923	-6.433	0.000e+00	0.00835	1.291	2.313
srt_002_04439	Cs ₈ Yb ₆	14	-0.776	-0.948	1.000e-06	0.00193	1.105	2.755

Table S11. The profile of generated materials with Small rhombitrihexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
srt_002_04451	I ₆ Mn ₆	12	-4.467	-4.921	-6.000e-06	0.00664	0.512	1.171
srt_002_04533	Ru ₉ Sn ₁₁	20	-5.797	-6.158	0.000e+00	0.00415	0.961	1.086
srt_002_04564	BaCo ₆ LiSn ₅	13	-4.6	-5.025	-1.500e-05	0.00627	1.278	3.117
srt_002_04594	BaBr ₂ Ge ₄ Mn ₆	13	-5.509	-5.92	-9.000e-06	0.00757	1.307	2.01
srt_002_04750	Cs ₇ Tb ₆	13	-1.641	-2.127	-6.200e-05	0.00949	3.901	4.072
srt_002_04827	Lu ₈ Ru ₆	14	-6.35	-6.73	-3.000e-06	0.0061	0.547	0.747
srt_002_04895	GeNi ₆ Sn ₅ Sr	13	-4.524	-4.635	-1.500e-05	0.00886	0.422	0.396
srt_002_04950	Co ₆ Sn ₈	14	-5.075	-5.116	0.000e+00	0.0094	0.272	0.277
srt_003_00038	AgAs ₂ Co ₇ GeSe ₇	18	-4.605	-5.103	-1.000e-06	0.00916	1.302	1.995
srt_003_00053	Mn ₇ Sn ₆	13	-5.543	-6.27	-5.000e-06	0.00762	1.103	2.519
srt_003_00066	EuFe ₆ Se ₂ Sn ₂ Sr ₃	14	-4.747	-5.158	-1.900e-05	0.00555	0.689	0.678
srt_003_00079	GeLiMn ₆ PtSb ₂ Sn ₄	15	-5.6	-5.875	-1.700e-05	0.00838	0.877	1.343
srt_003_00084	AlGe ₄ Ho ₂ Mn ₇ Sn ₂	16	-5.921	-6.342	8.400e-04	0.00613	0.796	1.422
srt_003_00148	Ga ₂ Ni ₆ Y ₆	14	-5.791	-5.922	1.000e-06	0.00896	0.71	0.817
srt_003_00197	KRu ₆ Se ₄ SiSmTe ₂	15	-5.666	-5.992	-3.000e-06	0.00536	1.549	1.988
srt_003_00221	K ₂ Ru ₇ Sn ₄	13	-5.284	-6.052	-5.000e-06	0.00442	1.529	1.655
srt_003_00239	I ₆ Ru ₆	12	-3.79	-4.923	4.000e-06	0.00912	0.787	3.117
srt_003_00262	Co ₆ Na ₈	14	-3.026	-3.277	-8.000e-06	0.00862	0.898	0.969
srt_003_00334	Cs ₇ Tb ₆	13	-1.733	-2.097	-1.000e-05	0.00799	2.425	3.2
srt_003_00454	CoEuGeMn ₆ PSn ₄ Zn	15	-5.587	-5.935	-3.000e-06	0.00618	0.824	1.036
srt_003_00459	Co ₆ Sn ₈	14	-4.907	-5.123	2.000e-06	0.00667	0.803	0.817
srt_003_00479	Co ₆ Ge ₄ Sn ₃	13	-5.179	-5.347	-5.000e-06	0.00941	0.205	0.728
srt_003_00485	Co ₈ EuGe ₆ LaSb	17	-5.471	-5.724	-1.000e-06	0.00915	1.037	1.454
srt_003_00491	Cs ₂ Ge ₂ Ru ₆ SeTe	12	-5.477	-5.978	0.000e+00	0.00333	1.743	1.277
srt_003_00629	Cs ₈ Yb ₆	14	-0.838	-0.953	-2.600e-05	0.00286	1.524	2.344
srt_003_00633	Al ₅ Ni ₆ SbSn ₂	14	-4.594	-4.716	-1.000e-06	0.00628	0.425	0.272
srt_003_00697	Cs ₇ Yb ₆	13	-0.837	-0.94	-2.600e-05	0.00284	0.873	3.457
srt_003_00737	ClCo ₆ O ₂ Tl ₃	12	-4.506	-4.953	-5.700e-05	0.00854	1.833	1.706
srt_003_00795	Cs ₆ SnYb ₆	13	-1.052	-1.252	0.000e+00	0.00703	1.133	4.055
srt_003_00869	BiGe ₅ HfMn ₇ Si	15	-6.462	-6.836	1.000e-05	0.00547	0.963	1.236
srt_003_00878	Cs ₇ Yb ₆	13	-0.81	-0.955	-1.100e-05	0.00405	1.567	2.702
srt_003_00939	Mg ₂ Ni ₆ Sn ₅ Tl	14	-3.866	-4.187	1.600e-05	0.00671	0.887	1.789
srt_003_01003	Cs ₅ Nd ₆ Rb	12	-1.928	-2.42	3.000e-06	0.00462	3.169	5.471
srt_003_01005	GaNi ₇ Sn ₆	14	-4.375	-4.727	0.000e+00	0.00731	0.743	0.902
srt_003_01019	Cs ₈ Nd ₆	14	-1.807	-2.134	2.000e-06	0.00169	1.974	3.055
srt_003_01123	Ge ₆ Mn ₆ Na ₂	14	-5.299	-5.784	-3.000e-05	0.00695	0.986	1.441
srt_003_01167	Cs ₇ Yb ₆	13	-0.858	-0.956	-9.000e-06	0.00518	1.4	2.251
srt_003_01169	LiMn ₆ Sn ₈	15	-5.319	-5.595	-1.000e-06	0.00585	1.153	1.043
srt_003_01181	Cd ₄ Ni ₆ PrS ₂ Si	14	-3.836	-4.11	-1.000e-05	0.00596	0.4	1.125
srt_003_01232	CaNi ₆ Sn ₇	14	-4.509	-4.571	-1.000e-06	0.00746	0.498	0.365
srt_003_01245	Co ₆ Cs ₄ Sn ₄	14	-3.978	-4.11	-1.000e-06	0.00845	0.697	0.768
srt_003_01254	Co ₆ Hf ₈	14	-8.53	-8.889	-8.000e-05	0.0067	0.572	0.607
srt_003_01283	Al ₂ CeNi ₆ PrSm ₂ Sn ₂	14	-4.836	-5.186	-6.000e-06	0.00754	1.058	2.03
srt_003_01309	BaGa ₇ Ni ₆	14	-3.929	-4.176	2.000e-06	0.00254	0.632	0.785
srt_003_01311	Dy ₈ Ni ₆	14	-4.864	-5.247	1.100e-05	0.00728	0.677	0.92
srt_003_01315	Ba ₂ Fe ₇ Ga ₆ Ge	16	-4.769	-5.102	-5.000e-06	0.00918	1.068	1.81
srt_003_01348	Ni ₆ SbSn ₇	14	-4.583	-4.659	0.000e+00	0.00791	0.427	1.057
srt_003_01358	Mn ₆ P ₂ Te ₆	14	-5.848	-6.007	-2.000e-06	0.00462	0.497	1.391
srt_003_01359	Mn ₆ Sn ₈	14	-5.58	-5.806	-1.000e-06	0.00335	0.614	0.86
srt_003_01374	Co ₆ Ga ₅ Yb ₃	14	-4.375	-4.543	-9.000e-06	0.00522	0.955	0.646
srt_003_01447	Ge ₃ Ni ₆ Tl ₂	11	-4.325	-4.572	0.000e+00	0.00777	0.749	0.478

Table S11. The profile of generated materials with Small rhombitrihexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
srt_003_01496	Co ₆ Sn ₇	13	-4.884	-5.12	-8.000e-06	0.00761	0.804	0.594
srt_003_01597	Co ₆ Sn ₇	13	-5.034	-5.103	-5.000e-06	0.00793	0.531	0.381
srt_003_01640	Al ₇ Ni ₆	13	-4.499	-5.006	-1.000e-05	0.00904	0.91	1.217
srt_003_01673	Cs ₈ Yb ₆	14	-0.808	-0.951	0.000e+00	0.00281	1.719	4.672
srt_003_01737	BiGe ₄ Ru ₆ SnTe	13	-5.747	-6.268	-4.000e-06	0.00599	0.773	0.648
srt_003_01754	AlGe ₄ La ₃ Mn ₆ Sr	15	-5.956	-6.329	7.000e-06	0.00515	0.955	1.066
srt_003_01785	Cs ₈ Yb ₆	14	-0.822	-0.952	-3.000e-06	0.00234	1.41	2.031
srt_003_01807	Na ₆ Ni ₆	12	-2.823	-3.184	2.000e-06	0.0087	1.167	1.072
srt_003_01815	Co ₇ Ge ₅ NdSn ₃	16	-5.287	-5.532	-3.000e-06	0.00809	1.157	1.465
srt_003_01856	CoNa ₂ Ni ₇ Si ₄	14	-4.899	-5.15	1.000e-06	0.00971	0.661	0.849
srt_003_01862	AuRu ₁₄ Sn ₅	20	-6.941	-7.41	0.000e+00	0.00719	0.277	0.491
srt_003_01863	Cs ₈ Nd ₆	14	-1.9	-2.136	0.000e+00	0.00186	1.299	2.209
srt_003_01882	Al ₃ BrCaGeRu ₇ SbTe	15	-5.725	-6.127	-3.000e-06	0.00473	0.647	0.832
srt_003_01899	Mn ₆ Sn ₈	14	-5.469	-5.778	3.000e-06	0.00632	0.734	0.763
srt_003_01941	KRu ₇ Sn ₇	15	-5.861	-6.086	1.000e-06	0.00625	0.443	1.035
srt_003_01956	BrGaNi ₆ Sn ₆	14	-4.178	-4.364	0.000e+00	0.00745	0.754	0.857
srt_003_02037	As ₂ Br ₂ GeNi ₆ Zn	12	-3.95	-4.301	1.000e-06	0.00503	0.656	1.468
srt_003_02062	Fe ₈ Si ₇ Y ₄	19	-6.669	-7.087	0.000e+00	0.00579	0.514	1.32
srt_003_02093	AlCe ₇ Mn ₆ Sm	15	-6.49	-6.883	0.000e+00	0.00996	0.968	1.283
srt_003_02100	Ca ₄ Ga ₄ Ni ₈	16	-4.014	-4.201	-2.000e-06	0.00892	0.656	0.818
srt_003_02117	GeRb ₄ Ru ₆ Sb ₄	15	-4.805	-5.306	-2.000e-06	0.00682	1.179	2.131
srt_003_02142	Al ₂ Ni ₈ Sn ₅	15	-4.557	-4.864	-2.800e-05	0.00864	0.839	1.277
srt_003_02192	Co ₇ Ga ₃ Nd ₃ Tb	14	-5.173	-5.614	6.000e-06	0.00999	1.045	1.7
srt_003_02239	KMn ₆ Sn ₇	14	-5.169	-5.547	-2.000e-06	0.00691	0.945	2.157
srt_003_02273	BaCo ₉ GeSb ₃	14	-5.44	-5.737	7.000e-06	0.00658	0.734	0.939
srt_003_02307	AlCa ₉ GaNi ₈	19	-3.543	-3.696	-5.000e-06	0.00652	0.87	1.44
srt_003_02309	Ni ₆ Sb ₃ SnSr ₄	14	-4.266	-4.384	-4.900e-05	0.00517	0.506	0.601
srt_003_02387	Co ₆ Sn ₈	14	-4.559	-5.123	-4.200e-05	0.00952	0.314	0.675
srt_003_02406	Co ₆ CsGe ₅	12	-4.837	-5.241	-1.000e-06	0.00538	0.754	1.212
srt_003_02409	Co ₆ Sn ₈	14	-4.724	-5.124	1.000e-06	0.00602	0.892	0.985
srt_003_02433	AlFe ₇ La ₄ Sn ₂ Tl	15	-5.79	-6.082	-1.900e-05	0.00714	1.244	1.423
srt_003_02455	EuK ₂ Ru ₆ Sn ₄ Sr	14	-5.182	-5.425	-4.000e-06	0.00436	0.818	0.582
srt_003_02474	Al ₉ Ru ₁₀	19	-6.507	-6.936	1.000e-05	0.00653	0.929	1.447
srt_003_02480	La ₄ Ni ₆ Sn ₃	13	-5.067	-5.308	3.000e-06	0.00866	1.399	1.529
srt_003_02500	Cs ₇ KNd ₆	14	-1.973	-2.159	-7.000e-06	0.00352	1.501	2.114
srt_003_02512	Cs ₈ Yb ₆	14	-0.74	-0.952	1.000e-05	0.00688	1.745	2.534
srt_003_02553	Ge ₃ Ni ₆ RuSmTh	12	-5.503	-5.984	0.000e+00	0.00707	1.381	1.081
srt_003_02560	Ga ₄ Na ₂ Ni ₆	12	-3.813	-3.979	3.000e-06	0.00731	0.801	0.419
srt_003_02581	Ni ₉ Rb ₂ Sn ₄	15	-4.057	-4.389	-9.000e-06	0.00575	1.393	1.387
srt_003_02604	Co ₆ Sn ₈	14	-4.752	-5.126	-2.100e-05	0.00532	0.844	0.58
srt_003_02634	Ru ₆ Sn ₆	12	-5.992	-6.325	-2.000e-06	0.00621	0.834	0.598
srt_003_02651	Fe ₁₀ Si ₈ TbZr	20	-6.868	-7.24	0.000e+00	0.00459	0.85	1.166
srt_003_02663	Ba ₂ Ga ₃ Ru ₇ Si	13	-6.032	-6.325	0.000e+00	0.0043	1.211	0.735
srt_003_02727	Cs ₈ Dy ₆	14	-1.743	-1.994	-1.000e-06	0.00416	1.158	1.867
srt_003_02795	AlGe ₉ Mn ₁₀	20	-6.279	-6.578	0.000e+00	0.00783	0.717	0.932
srt_003_02797	AlCo ₆ Sn ₄ Tl ₃	14	-4.53	-4.672	-2.000e-06	0.00935	0.723	0.98
srt_003_02805	Al ₄ LaRu ₈ Y	14	-6.778	-7.359	0.000e+00	0.00819	1.416	1.429
srt_003_02854	Ni ₆ Sn ₇	13	-4.501	-4.603	3.000e-06	0.0056	0.126	0.266
srt_003_02855	Ni ₈ Sn ₈	16	-4.661	-4.721	3.000e-06	0.0082	0.308	0.399
srt_003_02860	Cs ₇ Yb ₆	13	-0.827	-0.953	-2.000e-06	0.00177	1.81	3.189
srt_003_02871	Bi ₂ Eu ₄ GaNi ₇	14	-4.212	-4.411	-2.800e-05	0.00636	0.917	1.505

Table S11. The profile of generated materials with Small rhombitrihexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
srt_003_02961	LaMn ₆ Sn ₇	14	-5.837	-6.019	0.000e+00	0.00917	0.674	1.052
srt_003_03023	Cs ₈ Yb ₇	15	-0.795	-0.987	1.000e-05	0.00213	1.55	2.412
srt_003_03061	Co ₇ Ni ₂ Sn ₂ Sr ₂	13	-5.022	-5.317	3.000e-06	0.00644	0.717	1.968
srt_003_03069	Cs ₈ Nd ₆	14	-1.848	-2.133	-1.450e-04	0.0023	1.61	1.504
srt_003_03090	Cs ₈ Tb ₆	14	-1.711	-2.019	-3.600e-05	0.00732	1.843	2.993
srt_003_03211	EuLa ₃ Ru ₈ Sn ₃	15	-6.709	-6.936	0.000e+00	0.00748	0.735	1.261
srt_003_03256	Bi ₂ GeNi ₆ Tl ₂	11	-4.176	-4.429	-2.000e-06	0.0067	1.071	1.573
srt_003_03295	Co ₇ Ga ₂ Sn ₆	15	-4.858	-5.086	5.000e-06	0.00891	0.467	1.695
srt_003_03396	Cs ₄ Ge ₄ Ni ₆	14	-3.81	-3.973	1.000e-06	0.00469	1.409	1.169
srt_003_03400	Fe ₆ LaSn ₆ Sr	14	-5.342	-5.625	6.000e-06	0.00957	1.298	2.029
srt_003_03426	Al ₄ Co ₇ PdSc ₄	16	-5.991	-6.238	-3.400e-05	0.00875	0.822	1.059
srt_003_03428	Co ₆ Sn ₈	14	-4.924	-5.123	-3.000e-06	0.00585	0.862	1.745
srt_003_03497	Co ₈ NdY ₆	15	-6.553	-6.637	-2.600e-05	0.00985	0.355	0.38
srt_003_03586	Fe ₆ Ga ₈	14	-4.841	-5.097	-7.000e-06	0.00524	0.446	0.409
srt_003_03637	Cs ₂ Mn ₆ S ₇	15	-5.799	-6.272	-5.000e-06	0.00616	1.191	1.148
srt_003_03643	CaGaGe ₂ MgNi ₆ Sn ₂	13	-3.906	-4.43	-4.000e-06	0.00651	1.228	1.55
srt_003_03655	Ga ₄ Ru ₇ Sr ₄	15	-4.942	-5.535	4.000e-06	0.00584	1.283	2.184
srt_003_03657	Ga ₃ Mn ₆ Sn ₄ Sr	14	-5.075	-5.533	-3.000e-06	0.00557	0.97	2.038
srt_003_03693	Ru ₆ Sn ₆	12	-5.878	-6.188	-4.000e-06	0.00709	0.765	1.788
srt_003_03771	ErFe ₆ LaSn ₅ Ti	14	-5.676	-6.168	1.600e-05	0.00595	0.795	0.894
srt_003_03837	Nd ₂ Ru ₈ Sn ₄ Yb	15	-6.451	-6.737	0.000e+00	0.00596	0.437	0.994
srt_003_03855	Co ₆ Se ₇ Tl ₂	15	-4.824	-4.987	0.000e+00	0.0076	0.614	0.699
srt_003_03874	Fe ₇ Te ₇	14	-5.292	-5.51	1.000e-06	0.00876	0.853	1.871
srt_003_03899	Co ₆ KSn ₆	13	-4.848	-4.902	2.000e-06	0.00647	0.234	0.375
srt_003_04048	Cs ₈ Gd ₆	14	-1.78	-2.04	-1.900e-05	0.00365	1.576	1.435
srt_003_04174	Cs ₇ Gd ₆	13	-1.758	-2.121	-1.000e-06	0.00313	2.445	2.876
srt_003_04188	Al ₂ Ga ₃ Ni ₈ Y ₂	15	-5.023	-5.307	-2.400e-05	0.00682	1.208	2.035
srt_003_04192	BaCo ₆ NaSn ₃	11	-4.718	-4.959	-2.500e-05	0.00819	0.832	0.846
srt_003_04217	AgFe ₆ Se ₇	14	-5.272	-5.578	-1.000e-06	0.00645	0.933	1.17
srt_003_04266	Ce ₃ Ru ₁₁ SbSn	16	-7.708	-7.991	0.000e+00	0.00709	0.923	1.455
srt_003_04398	Al ₃ BaGeNi ₆ Sr	12	-4.355	-4.6	-2.400e-05	0.00369	0.955	0.492
srt_003_04402	Fe ₇ Ga ₅ Sn ₆	18	-4.746	-5.139	4.000e-06	0.00907	1.163	1.618
srt_003_04405	Bi ₂ Ge ₆ Mn ₆	14	-5.865	-6.079	4.000e-06	0.00991	0.827	0.759
srt_003_04411	Cs ₂ Ru ₆ Sn ₅	13	-5.247	-5.623	-3.000e-06	0.00577	0.696	1.319
srt_003_04435	Cs ₉ Dy ₆	15	-1.553	-1.906	-1.500e-05	0.00861	1.644	2.869
srt_003_04456	Ba ₂ Ru ₆ SeSnY ₄	14	-6.409	-6.696	-5.500e-05	0.00962	0.83	1.966
srt_003_04490	KMn ₆ S ₇	14	-6.249	-6.496	1.000e-06	0.00592	0.84	1.052
srt_003_04518	Co ₉ Ge ₂ Sr ₂	13	-5.459	-5.639	-1.700e-05	0.00651	0.585	0.406
srt_003_04520	Mn ₁₃ SbSn ₆	20	-6.415	-6.868	0.000e+00	0.00881	0.461	0.667
srt_003_04532	Ru ₆ Sn ₄ Tl ₂	12	-5.033	-5.971	-1.000e-06	0.00512	1.164	2.877
srt_003_04603	Cs ₇ Yb ₆	13	-0.735	-0.95	-6.000e-06	0.00184	1.848	2.792
srt_003_04640	CdCs ₈ Yb ₇	16	-0.774	-0.973	-5.000e-06	0.0025	0.84	2.949
srt_003_04719	Ni ₆ RuSn ₁₁	18	-4.386	-4.714	-1.000e-06	0.00943	0.574	1.056
srt_003_04729	Ba ₅ CdGa ₆ Ru ₇	19	-4.732	-4.884	3.000e-06	0.00585	0.544	1.637
srt_003_04736	Ni ₇ Pd ₂ Sn ₅	14	-4.738	-4.974	2.000e-06	0.00666	0.379	0.623
srt_003_04760	BaMn ₆ Sn ₇	14	-5.352	-5.776	-3.000e-06	0.00623	1.155	1.226
srt_003_04762	Al ₃ Ge ₂ La ₂ Mn ₈	15	-6.327	-6.808	0.000e+00	0.00957	1.071	1.667
srt_003_04792	Ni ₆ Sn ₈	14	-4.554	-4.636	0.000e+00	0.00736	0.336	0.256
srt_003_04827	Cs ₈ Gd ₆	14	-1.767	-2.036	2.000e-06	0.00247	1.641	3.309
srt_003_04840	Cs ₈ Yb ₆	14	-0.842	-0.953	-2.000e-06	0.00336	1.182	1.911
srt_003_04890	AuCs ₇ HgNd ₆	15	-1.975	-2.314	0.000e+00	0.00431	1.651	3.162

Table S11. The profile of generated materials with Small rhombitrihexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
srt_003_05002	Ge ₆ Ru ₈ Y ₃	17	-6.841	-7.323	0.000e+00	0.00804	0.825	1.277
srt_003_05047	Ru ₆ Sn ₈	14	-5.891	-6.032	-1.200e-05	0.00591	0.321	0.428
srt_004_00016	Co ₆ Na ₆ Pr	13	-3.351	-3.776	-1.900e-05	0.00662	1.016	1.479
srt_004_00065	Ba ₄ Ni ₆ Sn ₄	14	-4.073	-4.262	-2.300e-05	0.00974	0.714	0.648
srt_004_00205	Cs ₈ Gd ₆	14	-1.663	-2.036	-3.000e-05	0.00198	1.796	2.509
srt_004_00215	Al ₂ Fe ₁₀ La ₄ Sb ₂	18	-5.934	-6.484	0.000e+00	0.00835	1.553	1.268
srt_004_00231	Mn ₆ Se ₆ Tl ₂	14	-5.518	-5.826	-1.100e-05	0.00751	0.448	0.977
srt_004_00248	GeK ₃ Ru ₇ Sn ₅ Te	17	-4.974	-5.366	-5.000e-06	0.00533	0.416	1.067
srt_004_00273	Ba ₂ Ni ₆ Sn ₃	11	-4.35	-4.564	-6.000e-06	0.00913	1.191	1.405
srt_004_00311	GeNi ₆ Sn ₇	14	-4.434	-4.676	1.000e-06	0.0044	0.295	2.374
srt_004_00328	Co ₆ Li ₂ Sn ₄ Sr	13	-4.519	-4.804	-1.000e-06	0.00951	1.035	1.749
srt_004_00370	Ru ₆ Sn ₆ Sr	13	-5.829	-6.06	-8.000e-06	0.00863	1.189	1.628
srt_004_00411	Ru ₆ Se ₇ Sr	14	-5.828	-6.065	-9.000e-06	0.00637	1.131	1.201
srt_004_00437	Cs ₆ Yb ₆	12	-0.824	-0.937	0.000e+00	0.00137	1.32	3.646
srt_004_00545	Ni ₆ Sn ₈	14	-4.535	-4.631	-2.000e-06	0.00927	0.453	0.436
srt_004_00635	Co ₇ Li ₃ Si ₃ Sn ₂	15	-5.036	-5.358	-4.000e-06	0.00708	0.407	1.381
srt_004_00685	Ni ₆ Sn ₈	14	-4.47	-4.567	-2.000e-06	0.00757	0.507	1.811
srt_004_00736	Ni ₆ Sn ₆	12	-4.353	-4.785	3.000e-06	0.00653	1.402	1.085
srt_004_00739	Ni ₁₂ Sn ₈	20	-4.586	-4.944	-1.100e-05	0.00935	0.859	1.948
srt_004_00747	Ni ₆ Se ₄ Te ₂	12	-4.34	-4.591	-1.000e-06	0.00471	0.387	0.486
srt_004_00767	As ₆ Fe ₉ SbTi	17	-6.335	-6.684	2.000e-05	0.00788	0.543	1.0
srt_004_00783	Ba ₃ Co ₆ Sn ₅	14	-4.568	-4.845	-3.000e-06	0.00457	0.902	1.127
srt_004_00815	Al ₅ EuGdNi ₇	14	-4.573	-4.918	-8.600e-05	0.00847	0.956	2.619
srt_004_00880	Rb ₂ Ru ₆ Sn ₆	14	-4.941	-5.516	-6.000e-06	0.00553	0.682	0.894
srt_004_00970	Mn ₁₀ Si ₁₀	20	-6.908	-7.298	0.000e+00	0.0054	0.619	0.611
srt_004_00998	GaNi ₇ Zr ₇	15	-6.767	-7.038	0.000e+00	0.00879	0.878	1.517
srt_004_01067	Ca ₈ Ru ₆	14	-4.515	-4.99	5.000e-06	0.00459	0.987	0.926
srt_004_01087	Ni ₇ Sn ₅ Sr	13	-4.302	-4.709	-2.300e-05	0.00939	1.206	1.995
srt_004_01139	As ₃ Co ₆ Na ₄ Ni	14	-4.513	-4.672	-6.000e-06	0.00518	0.815	0.6
srt_004_01218	Ni ₆ Sn ₈	14	-4.342	-4.633	-1.000e-06	0.00652	0.527	0.459
srt_004_01220	Ni ₆ Sn ₇	13	-4.457	-4.561	0.000e+00	0.0058	0.431	0.46
srt_004_01266	Eu ₈ Ru ₆	14	-4.886	-5.096	-1.600e-05	0.00659	0.759	1.09
srt_004_01269	Cs ₂ Ni ₆ SeSn ₂ Te ₂	13	-3.948	-4.137	2.000e-06	0.00779	0.512	0.802
srt_004_01276	Cs ₇ Yb ₆	13	-0.743	-0.953	-1.000e-06	0.00206	1.682	2.234
srt_004_01336	GaLa ₃ Ni ₆ Si ₃ Sm	14	-5.332	-5.608	-4.000e-06	0.00846	0.782	0.777
srt_004_01393	Co ₇ Sn ₈	15	-4.896	-5.215	-3.000e-06	0.00838	0.567	0.58
srt_004_01417	Cs ₇ Yb ₆	13	-0.76	-0.954	-2.000e-06	0.00227	1.78	2.086
srt_004_01431	Cs ₇ Dy ₆	13	-1.819	-2.077	3.000e-06	0.00275	1.926	4.597
srt_004_01447	Fe ₆ Sb ₄ Sr ₄	14	-5.1	-5.236	-1.000e-06	0.00621	0.717	0.44
srt_004_01536	Fe ₆ GeLaSn ₆	14	-5.31	-5.723	-1.000e-06	0.00443	0.986	0.902
srt_004_01565	Mn ₆ Se ₅ Tl ₂	13	-5.37	-5.859	-4.100e-05	0.00612	0.77	1.353
srt_004_01603	Ba ₃ Co ₆ Sn ₆	15	-4.732	-4.794	0.000e+00	0.00883	0.302	0.377
srt_004_01612	KNi ₆ Sn ₇	14	-4.474	-4.497	4.000e-06	0.00705	0.136	0.635
srt_004_01629	Ru ₇ Sb ₃ Sn ₅	15	-5.947	-6.254	2.000e-06	0.00593	0.559	1.058
srt_004_01646	Co ₆ Cs ₂ Se ₄	12	-4.41	-4.945	-1.100e-05	0.00466	1.523	0.534
srt_004_01670	Cs ₈ Tb ₆	14	-1.75	-2.015	-2.000e-05	0.00442	1.534	5.208
srt_004_01692	Rb ₄ Ru ₆ Se ₅	15	-4.888	-5.18	5.000e-06	0.00484	0.667	0.514
srt_004_01715	Co ₇ Ge ₇ HfU	16	-6.134	-6.485	0.000e+00	0.00787	0.896	2.216
srt_004_01723	GeMn ₈ Sn ₇	16	-5.927	-6.195	-6.000e-06	0.0058	0.6	1.687
srt_004_01801	Co ₆ Cs ₂ La ₄	12	-4.713	-5.157	-1.100e-05	0.00698	1.988	1.886
srt_004_01884	Co ₉ Sb ₂ Sn ₄ Sr ₂	17	-4.825	-5.35	8.000e-06	0.00626	1.595	2.033

Table S11. The profile of generated materials with Small rhombitrihexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
srt_004_01945	Cs ₆ Yb ₈	14	-0.857	-1.012	-4.000e-05	0.00322	1.4	2.586
srt_004_01946	Cs ₅ Nd ₆	11	-2.163	-2.466	1.000e-06	0.00288	0.9	3.16
srt_004_01965	Na ₃ Ru ₆ Sn ₅	14	-5.045	-5.399	-6.000e-06	0.00825	0.995	1.332
srt_004_01968	Al ₂ Ce ₆ Co ₆	14	-6.083	-6.285	-1.000e-06	0.00695	0.535	0.518
srt_004_01971	GeNi ₆ Te ₇	14	-4.091	-4.371	-3.000e-06	0.00637	0.298	0.555
srt_004_01991	Ni ₇ Sn ₈	15	-4.579	-4.701	0.000e+00	0.00508	0.126	0.294
srt_004_01992	CoMn ₇ NiSn ₁₁	20	-4.998	-5.627	0.000e+00	0.00769	1.052	1.391
srt_004_02022	Ru ₇ Sn ₈	15	-5.708	-6.224	-3.000e-06	0.0052	0.917	1.533
srt_004_02062	EuFe ₆ Sn ₇	14	-5.255	-5.462	-7.000e-06	0.00498	0.75	1.707
srt_004_02074	Co ₆ Sn ₈	14	-5.066	-5.129	-1.000e-06	0.00553	0.289	0.207
srt_004_02087	Al ₃ Ce ₅ Ni ₇	15	-5.502	-5.637	2.000e-06	0.00966	0.818	1.818
srt_004_02109	Ni ₆ Se ₆	12	-4.431	-4.707	-6.000e-06	0.00805	0.806	2.464
srt_004_02112	Co ₆ Sn ₅ Sr ₄	15	-4.373	-4.655	-6.000e-06	0.00759	1.067	1.205
srt_004_02135	Cs ₆ Yb ₆	12	-0.764	-0.943	-8.000e-06	0.00344	1.574	3.273
srt_004_02172	AgCo ₆ Sn ₆ Tm	14	-4.909	-5.125	2.000e-06	0.00458	0.599	0.623
srt_004_02229	Co ₆ Cs ₂ SeSn ₅ Y	15	-4.615	-4.882	2.000e-06	0.00951	0.612	1.422
srt_004_02269	Cs ₈ Nd ₆	14	-1.791	-2.137	1.500e-05	0.00296	1.927	3.02
srt_004_02291	Ni ₆ Sn ₇ Sr	14	-4.45	-4.588	-3.300e-05	0.00812	0.665	0.409
srt_004_02319	As ₃ Ge ₅ Ni ₆ Yb	15	-4.616	-4.933	1.000e-06	0.00907	1.376	1.502
srt_004_02381	BaGa ₆ KNi ₆	14	-3.837	-4.05	-7.000e-06	0.00837	1.126	1.302
srt_004_02414	Co ₁₀ Ge ₃ La ₃ SbSn	18	-5.894	-6.08	0.000e+00	0.00753	0.663	2.311
srt_004_02431	Cs ₈ Yb ₆	14	-0.843	-0.953	0.000e+00	0.00216	1.562	2.38
srt_004_02449	Ni ₆ Sn ₈	14	-4.557	-4.631	-1.200e-05	0.00839	0.235	0.298
srt_004_02510	Co ₆ Sn ₇	13	-5.025	-5.096	0.000e+00	0.00909	0.351	0.343
srt_004_02538	Ni ₁₀ SbSn ₉	20	-4.272	-4.737	2.000e-06	0.00663	0.927	2.003
srt_004_02592	Co ₆ PdSn ₁₂	19	-4.704	-4.9	-9.000e-06	0.00517	0.791	1.43
srt_004_02648	BaCo ₆ EuSn ₄	12	-4.841	-5.192	-3.000e-06	0.00862	1.368	0.993
srt_004_02670	Ga ₂ Ni ₇ Th ₂ V ₂	13	-5.867	-6.202	-7.000e-06	0.00879	1.051	1.316
srt_004_02724	La ₅ NiRu ₁₀ Sn ₃	19	-6.891	-7.083	0.000e+00	0.00755	0.42	0.908
srt_004_02743	Cs ₆ Yb ₆	12	-0.795	-0.965	-5.000e-06	0.00217	1.541	3.297
srt_004_02769	AlCaLa ₂ P ₃ Ru ₈ Si	16	-6.893	-7.326	0.000e+00	0.00556	0.835	0.634
srt_004_02777	Al ₁₀ GeMn ₇ Nd ₂	20	-5.292	-5.793	1.000e-05	0.00464	0.436	0.784
srt_004_02842	Ba ₂ Ni ₆ Sn ₆	14	-4.42	-4.546	-1.300e-05	0.00779	0.935	1.604
srt_004_02848	Mg ₇ Ni ₇ Sr	15	-3.24	-3.432	-2.600e-05	0.00592	1.245	2.479
srt_004_02856	Cs ₈ Yb ₆	14	-0.85	-0.953	-9.000e-06	0.0024	1.594	2.64
srt_004_02871	Ge ₃ La ₅ Mn ₇ Rh	16	-6.562	-6.857	0.000e+00	0.00759	0.774	1.184
srt_004_02878	Bi ₂ ErInMo ₂ Ni ₁₀	16	-5.491	-5.669	3.000e-06	0.0055	0.27	0.882
srt_004_02887	Cs ₅ Dy ₆ Pb ₂	13	-2.478	-2.779	0.000e+00	0.00501	2.402	2.037
srt_004_02925	As ₄ Co ₆ GeK ₂	13	-5.195	-5.252	-3.400e-05	0.00963	0.571	0.485
srt_004_03012	Al ₃ Co ₆ KNa ₂	12	-4.117	-4.496	1.000e-06	0.00644	1.103	3.172
srt_004_03031	Al ₃ La ₈ PbRu ₆	18	-6.102	-6.266	0.000e+00	0.00585	0.265	0.883
srt_004_03160	Ba ₂ Ge ₄ Ni ₆	12	-4.543	-4.779	-4.000e-06	0.00782	0.592	1.663
srt_004_03165	Ce ₂ Ge ₄ Ru ₈ Sn	15	-6.807	-7.283	1.000e-05	0.00567	0.806	0.73
srt_004_03192	Ba ₂ CuMn ₆ Se ₆	15	-5.214	-5.749	-1.100e-05	0.00528	0.971	1.512
srt_004_03249	As ₈ Mn ₆	14	-6.214	-6.583	-1.600e-05	0.00344	0.792	1.682
srt_004_03277	Cs ₈ Yb ₆	14	-0.836	-0.953	-5.000e-06	0.00358	1.547	2.888
srt_004_03281	AsGeLiRu ₉ Sn ₃	15	-6.436	-6.961	0.000e+00	0.00571	0.946	1.193
srt_004_03286	Al ₃ Co ₆ Ge ₄ Ho	14	-5.28	-5.566	1.000e-06	0.00922	0.9	0.691
srt_004_03292	Cs ₉ Yb ₆	15	-0.791	-0.94	-6.000e-06	0.00337	0.998	2.751
srt_004_03294	Mn ₆ P ₈	14	-6.683	-7.195	0.000e+00	0.00862	0.666	0.954
srt_004_03348	Ba ₂ Ga ₄ Ni ₆	12	-4.094	-4.271	-1.000e-06	0.00734	1.254	0.805

Table S11. The profile of generated materials with Small rhombitrihexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
srt_004_03349	Cs ₈ Nd ₆	14	-1.935	-2.136	-1.000e-06	0.00268	1.617	2.149
srt_004_03470	Ni ₆ Sn ₇	13	-4.248	-4.622	-1.100e-05	0.00804	0.808	0.816
srt_004_03477	Ga ₅ LiNi ₆ Sn	13	-3.919	-4.175	-9.000e-06	0.00641	0.968	2.41
srt_004_03489	BaMn ₆ Sn ₆	13	-5.581	-5.854	0.000e+00	0.00642	0.645	0.55
srt_004_03529	Fe ₆ Se ₇ Sr ₂	15	-5.13	-5.59	1.000e-06	0.00637	0.615	1.095
srt_004_03547	Al ₃ AsCa ₂ Fe ₆ La ₂	14	-5.413	-5.727	-6.000e-06	0.0065	0.918	0.565
srt_004_03552	Cs ₈ Tb ₆	14	-1.567	-2.019	-4.900e-05	0.00706	2.023	3.575
srt_004_03586	Ni ₆ Sn ₈	14	-4.35	-4.629	1.000e-06	0.00678	0.389	0.55
srt_004_03625	Co ₆ Hg ₈	14	-2.433	-2.678	4.000e-06	0.00498	0.807	0.67
srt_004_03636	Co ₆ Ga ₄ Tl ₄	14	-3.995	-4.267	-2.400e-05	0.00659	0.725	0.543
srt_004_03643	Mn ₆ Sn ₈	14	-5.657	-5.803	-1.000e-06	0.00932	0.837	1.096
srt_004_03751	Bi ₃ Ge ₃ Ru ₆ Tl ₂	14	-5.508	-5.848	0.000e+00	0.00739	1.018	0.645
srt_004_03766	Co ₆ Ge ₄ Sn ₄	14	-4.869	-5.349	-1.000e-06	0.00737	0.229	0.643
srt_004_03828	Ni ₁₀ Sn ₈ Zn	19	-4.397	-4.627	-2.000e-06	0.00759	0.355	1.381
srt_004_03919	NaNi ₆ Sn ₃ Zn	11	-4.002	-4.32	-3.000e-06	0.00886	1.056	2.206
srt_004_03933	Co ₆ Sn ₈	14	-4.582	-5.128	2.000e-06	0.00561	0.221	0.252
srt_004_03934	Ba ₂ Co ₆ Ga ₄	12	-4.583	-4.857	-1.000e-06	0.0084	1.207	0.949
srt_004_04031	Ba ₄ Co ₆ Sn ₄	14	-4.581	-4.735	-3.000e-06	0.00395	1.08	0.838
srt_004_04080	La ₇ Ru ₆ Tl	14	-6.571	-6.692	-2.000e-06	0.00553	0.592	1.132
srt_004_04134	AgLiNi ₆ Sn ₅	13	-4.089	-4.406	0.000e+00	0.00494	1.655	1.346
srt_004_04166	GaNi ₆ Sn ₅	12	-4.383	-4.709	2.000e-06	0.00706	1.549	0.94
srt_004_04205	Ga ₅ LaNi ₆ U ₃	15	-5.603	-5.942	-1.100e-05	0.00875	0.634	1.726
srt_004_04222	BaBi ₂ Ga ₆ LaRu ₆ SnSr	18	-5.08	-5.299	-3.000e-06	0.00685	1.12	2.278
srt_004_04254	Mn ₈ Sb ₄ SnSr ₂	15	-5.935	-6.308	-8.000e-06	0.00603	1.083	1.021
srt_004_04257	Ce ₂ Ge ₆ Mn ₇ Pd	16	-6.424	-6.807	0.000e+00	0.00936	0.597	1.305
srt_004_04270	BaCo ₈ GeSn ₃	13	-5.158	-5.53	-1.000e-06	0.00488	0.966	0.994
srt_004_04297	La ₂ Ru ₁₂	14	-7.964	-8.4	0.000e+00	0.00672	0.603	1.107
srt_004_04343	Co ₆ Ga ₂ Ge ₂ Nd ₃	13	-5.447	-5.707	0.000e+00	0.00525	0.698	1.638
srt_004_04369	Ni ₆ Sn ₁₀	16	-3.4	-4.485	-1.000e-05	0.00681	0.753	1.694
srt_004_04463	AlBa ₂ Co ₇ Ge ₆	16	-5.125	-5.344	0.000e+00	0.00758	0.922	0.629
srt_004_04466	Ba ₄ Ru ₆ Sn ₄	14	-5.128	-5.682	2.000e-06	0.00453	1.196	0.988
srt_004_04530	Co ₉ EuIn ₂ Sm	13	-5.109	-5.628	2.100e-05	0.00984	0.996	1.514
srt_004_04594	AgGa ₂ Ru ₆ Se ₆	15	-5.414	-5.707	-3.000e-06	0.00488	0.839	0.9
srt_004_04638	Cs ₈ Tb ₆	14	-1.644	-2.02	-5.800e-05	0.00581	2.167	3.293
srt_004_04643	Cs ₈ Yb ₆	14	-0.85	-0.953	1.000e-06	0.00251	1.598	2.032
srt_004_04644	MgNi ₉ Sb ₅ Sn ₂	17	-4.562	-4.748	-1.500e-05	0.00994	0.453	1.65
srt_004_04665	Ru ₆ Sb ₂ Sn ₅	13	-5.746	-6.159	3.000e-06	0.00528	0.668	0.478
srt_004_04719	Co ₁₀ Te ₁₀	20	-4.662	-5.033	2.000e-05	0.00683	0.69	1.208
srt_004_04728	Ga ₇ La ₃ Ru ₇	17	-5.832	-6.136	0.000e+00	0.00371	0.915	1.246
srt_004_04758	Cs ₈ Yb ₆	14	-0.832	-0.953	4.000e-06	0.00225	1.245	1.865
srt_004_04828	Ni ₆ PRb ₂ Se ₅	14	-4.416	-4.568	2.000e-06	0.00757	0.536	0.701
srt_004_04861	Cs ₆ Nd ₆	12	-1.942	-2.403	4.000e-06	0.00383	3.445	3.629
srt_004_04877	Al ₃ AsCo ₇ Pr ₂	13	-5.579	-5.895	3.000e-06	0.00964	0.555	0.857
srt_004_04915	Ru ₁₀ SbSi ₄ Zr ₅	20	-8.153	-8.432	-1.000e-05	0.00691	0.654	0.945
srt_004_04939	Cs ₃ Ni ₆ Sn ₄	13	-3.744	-3.92	-6.000e-06	0.00753	0.751	1.638
srt_004_04964	Cs ₇ Yb ₆	13	-0.785	-0.95	-7.000e-06	0.0043	2.769	5.101
srt_005_00060	AgFe ₉ Ge ₄ La ₂ Ta	17	-6.333	-6.853	0.000e+00	0.00417	1.361	1.173
srt_005_00069	Ba ₂ Ga ₃ Ru ₈	13	-6.26	-6.484	0.000e+00	0.00687	0.782	0.982
srt_005_00107	Co ₆ Er ₅ InSbSn ₂	15	-5.276	-5.5	-1.000e-06	0.00725	0.895	0.92
srt_005_00140	Co ₆ Si ₇ UZr ₃	17	-6.864	-7.374	0.000e+00	0.00597	0.722	1.478
srt_005_00143	Cs ₂ Ge ₃ Ru ₆ Sn	12	-5.45	-5.93	-5.000e-06	0.0051	1.271	0.897

Table S11. The profile of generated materials with Small rhombitrihexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
srt_005_00149	Co ₇ Ge ₆ Pr ₂	15	-5.562	-5.948	-1.400e-05	0.00795	0.718	1.746
srt_005_00160	Cs ₆ Yb ₆	12	-0.793	-1.002	-3.900e-05	0.00412	3.115	3.297
srt_005_00162	CaGe ₃ Ni ₁₀ ReSn ₃	18	-5.307	-5.302	-1.000e-06	0.00857	0.726	1.875
srt_005_00203	Co ₆ Ge ₂ LiSn ₆	15	-4.935	-5.022	-7.000e-06	0.00774	0.173	0.302
srt_005_00235	Al ₄ Co ₆ Cs ₂	12	-4.35	-4.466	-1.000e-06	0.0035	0.394	0.355
srt_005_00237	Cs ₃ Rb ₃ Yb ₆	12	-0.818	-0.977	8.000e-06	0.00269	1.398	2.635
srt_005_00277	Co ₆ Ga ₅ Tl ₂	13	-4.268	-4.584	-6.000e-06	0.00668	0.925	1.069
srt_005_00308	Mn ₆ Sn ₅ Sr ₂	13	-5.444	-5.747	0.000e+00	0.00421	0.494	2.49
srt_005_00322	GaNi ₆ Sn ₅	12	-4.208	-4.729	-2.000e-06	0.00466	0.357	1.767
srt_005_00365	Cs ₇ Dy ₆	13	-1.681	-2.129	-2.700e-05	0.00693	3.403	3.738
srt_005_00384	EuGdNi ₆ Sn ₆	14	-4.685	-4.764	-9.000e-06	0.0098	0.225	0.283
srt_005_00414	CsFe ₆ SSe ₆	14	-5.6	-5.722	-1.500e-05	0.00746	0.348	1.266
srt_005_00467	Cs ₇ Yb ₇	14	-0.791	-0.974	-1.000e-06	0.0015	1.175	1.84
srt_005_00502	Co ₆ Sn ₆ Sr	13	-4.801	-5.091	-4.000e-06	0.0049	0.401	0.895
srt_005_00510	Ni ₆ Sn ₅ Sr ₂	13	-4.243	-4.417	-2.300e-05	0.00942	0.736	1.268
srt_005_00537	Ga ₂ GeNi ₇ Tl ₂	12	-4.071	-4.433	-3.000e-06	0.00987	0.671	1.476
srt_005_00625	Co ₇ Ge ₃ Si ₂ Tb ₂	14	-5.806	-6.28	-1.100e-05	0.00725	1.278	1.335
srt_005_00635	Al ₃ Ru ₇ SnTb ₄	15	-6.009	-6.755	0.000e+00	0.00626	1.257	1.654
srt_005_00653	EuGaGdNi ₆ Sn ₆	15	-4.327	-4.583	-9.000e-06	0.00651	0.566	0.434
srt_005_00661	Al ₉ Co ₈ La ₂	19	-5.332	-5.429	-1.600e-04	0.00991	0.504	0.306
srt_005_00664	Al ₄ AuLu ₅ NdRu ₆ Sn ₃	20	-5.52	-5.958	0.000e+00	0.00788	0.821	1.367

Table S12. The profile of generated materials with Snub hexagonal lattice structures after DFT relaxation

Index	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
snh_000_00034	CeCo ₆ Sn ₇	14	-4.813	-5.407	-8.000e-06	0.00849	0.287	0.659
snh_000_00052	Al ₄ Ba ₂ Ni ₆ Sn ₂ Sr	15	-4.177	-4.301	8.000e-06	0.00862	0.15	0.464
snh_000_00086	Mn ₆ Sn ₈	14	-5.511	-5.771	-1.000e-06	0.00659	0.669	1.586
snh_000_00136	Ni ₆ Sn ₄ Sr	11	-4.235	-4.66	-2.000e-06	0.00649	0.726	1.546
snh_000_00158	Ce ₂ Ni ₁₁ Si ₃	16	-5.75	-5.944	-2.100e-05	0.00642	0.544	0.77
snh_000_00175	Ni ₇ Tl ₂ Zn ₂	11	-3.668	-3.996	4.000e-06	0.00611	0.98	0.685
snh_000_00183	Ni ₁₁ Sn ₄	15	-4.776	-5.127	1.000e-06	0.00821	0.593	1.899
snh_000_00195	Co ₈ Sn ₈	16	-5.147	-5.373	1.000e-06	0.0064	0.604	1.59
snh_000_00206	Ru ₆ Sn ₈	14	-5.643	-6.027	-1.900e-05	0.0057	0.775	2.233
snh_000_00211	Mn ₆ Sn ₈	14	-5.272	-5.767	0.000e+00	0.00806	0.836	1.42
snh_000_00213	Al ₃ GeMn ₇ PPtSbSc	15	-6.267	-6.756	0.000e+00	0.0041	0.891	1.208
snh_000_00214	Co ₁₄ Si ₅ Sn	20	-6.403	-6.591	-5.000e-05	0.00804	0.2	0.364
snh_000_00258	GeMn ₆ Sn ₆	13	-5.55	-6.016	0.000e+00	0.00799	0.936	1.733
snh_000_00312	Ni ₇ Sn ₇	14	-4.109	-4.709	-1.000e-06	0.00724	0.691	0.88
snh_000_00324	Co ₆ ErGeIn ₈	16	-3.904	-4.368	-6.000e-06	0.00914	1.082	1.014
snh_000_00403	AgNi ₉ Sn ₃ Tb	14	-4.667	-4.931	2.000e-06	0.00653	0.392	0.571
snh_000_00409	Ni ₉ Sn ₃ Tl ₂	14	-4.223	-4.546	-1.000e-06	0.00973	1.011	1.025
snh_000_00427	Mn ₆ Sn ₁₁	17	-3.809	-5.315	-3.500e-05	0.00874	1.211	1.93
snh_000_00506	Al ₃ Ni ₈ Sn	12	-4.741	-5.18	-8.000e-06	0.00629	0.591	0.933
snh_000_00527	Ni ₉ Sn ₈	17	-4.45	-4.784	-1.000e-06	0.00561	0.726	0.902
snh_000_00564	AlGaKNi ₈ Sn	12	-4.315	-4.624	-3.000e-06	0.0042	0.723	1.618
snh_000_00578	Ni ₆ Sn ₂ Te ₅	13	-4.137	-4.468	7.000e-06	0.00881	0.868	1.545
snh_000_00617	Cs ₅ Yb ₆	11	-0.887	-0.966	2.000e-06	0.00364	0.663	1.776
snh_000_00621	BiEu ₂ Ga ₃ Ni ₆	12	-4.182	-4.429	-1.000e-06	0.00712	0.693	1.429
snh_000_00674	CeRu ₉ Sn ₃	13	-7.122	-7.554	0.000e+00	0.00432	0.442	0.567
snh_000_00689	Co ₆ La ₈	14	-5.701	-5.89	-3.000e-06	0.00749	1.056	1.039
snh_000_00745	AlCeCo ₆ GeNdSr	11	-5.321	-5.796	-1.700e-05	0.0095	0.943	1.489
snh_000_00835	Fe ₆ Ga ₆ Sr	13	-4.894	-5.184	-1.200e-05	0.00764	0.717	1.154
snh_000_00872	Cs ₄ Nd ₆	10	-2.547	-2.624	0.000e+00	0.00407	0.593	0.446
snh_000_00934	Co ₆ Sn ₇ Sr ₂	15	-4.342	-4.864	-4.000e-05	0.00691	0.631	1.214
snh_000_00956	Co ₇ SbSn ₃ SrTm	13	-5.055	-5.425	-1.000e-06	0.00764	1.008	1.297
snh_000_00969	Co ₇ Ga ₄ Sb ₂ Zr	14	-5.339	-5.594	2.000e-06	0.00665	0.852	1.072
snh_000_01015	Co ₆ Sn ₈ Sr ₂	16	-4.65	-4.784	-1.200e-05	0.0066	0.323	0.877
snh_000_01017	Al ₂ Co ₆ Na ₂	10	-4.434	-4.961	-1.000e-06	0.00979	0.708	0.835
snh_000_01085	La ₈ Ni ₇	15	-5.167	-5.415	2.000e-06	0.00633	1.36	2.87
snh_000_01106	Cs ₃ Ru ₆	9	-4.96	-5.583	-2.000e-06	0.00773	1.111	1.254
snh_000_01129	Mn ₆ Rb ₄ Sn ₄	14	-4.544	-4.801	-6.000e-05	0.0077	1.006	1.093
snh_000_01270	Ge ₂ Mn ₆ Sn ₆	14	-5.576	-5.883	2.000e-06	0.00534	0.849	1.794
snh_000_01295	Fe ₆ La ₃ Sn ₅	14	-5.812	-6.045	-1.100e-05	0.00717	0.609	0.88
snh_000_01325	As ₇ Fe ₇	14	-6.002	-6.379	-1.100e-05	0.00364	0.495	1.438
snh_000_01336	Er ₄ Ge ₂ Ni ₇ SSe	15	-5.076	-5.499	1.000e-06	0.00973	0.941	1.323
snh_000_01363	Mn ₆ Rb ₂ Sb ₄ Sn	13	-5.096	-5.741	-2.300e-05	0.00834	1.759	1.981
snh_000_01386	Cs ₈ Yb ₆	14	-0.851	-0.95	1.300e-05	0.00376	1.252	2.213
snh_000_01505	Ru ₆ Se ₆	12	-5.899	-6.359	-6.000e-06	0.00497	0.92	0.982
snh_000_01576	Co ₆ Pr ₂ Sn ₂	10	-5.481	-5.958	1.900e-05	0.00941	0.887	2.346
snh_000_01595	CaGa ₅ Ni ₆	12	-4.096	-4.369	-4.000e-06	0.00512	0.496	1.912
snh_000_01692	Cs ₂ Ru ₆ Se ₄	12	-5.506	-5.908	-3.000e-06	0.00801	0.81	0.776
snh_000_01697	EuNi ₁₀ Sn ₃	14	-4.741	-5.009	-1.000e-06	0.00844	0.623	1.193
snh_000_01818	Ge ₅ Ni ₇ Sr ₂	14	-4.478	-4.834	0.000e+00	0.00601	0.648	1.037
snh_000_01877	AgBiGaNaRu ₆ SiSnYZn	14	-5.275	-5.812	-2.300e-05	0.00858	0.993	2.346
snh_000_01903	AlBaRu ₇ Sn ₄	13	-6.2	-6.47	0.000e+00	0.00535	0.542	1.951
snh_000_01928	AlLaNi ₁₂	14	-5.161	-5.407	-1.840e-04	0.00926	0.57	0.777

Table S12. The profile of generated materials with Snub hexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
snh_000_01938	CaNi ₆ Sn ₄	11	-4.447	-4.709	-1.100e-05	0.00848	1.095	1.192
snh_000_01949	Co ₆ Ga ₄ Sr ₄	14	-4.159	-4.375	-1.900e-05	0.00965	0.674	0.622
snh_000_01999	Ag ₃ Al ₃ LaRu ₆ Sn	14	-5.433	-5.931	-2.000e-06	0.00671	0.758	1.489
snh_000_02055	KNi ₆ Sn ₅	12	-4.242	-4.448	0.000e+00	0.00687	0.791	1.875
snh_000_02081	Ni ₇ PrSn ₄	12	-4.843	-5.024	0.000e+00	0.00874	1.087	1.268
snh_000_02166	Co ₇ GaNd ₆	14	-5.568	-5.765	-5.000e-06	0.00913	0.563	1.173
snh_000_02170	Ni ₆ Sn ₈	14	-4.496	-4.632	-5.000e-06	0.00982	0.512	1.262
snh_000_02190	Ce ₅ Ru ₉	14	-7.617	-8.132	-1.000e-05	0.00938	0.734	2.382
snh_000_02242	Ni ₉ Sn ₅ Sr ₂	16	-4.223	-4.634	-6.000e-06	0.00935	0.776	1.633
snh_000_02322	Co ₇ Ge ₄ La ₃	14	-5.798	-6.087	-3.800e-05	0.00868	0.776	0.601
snh_000_02388	BaMn ₆ Sn ₆	13	-5.227	-5.868	-8.000e-06	0.00591	0.849	1.476
snh_000_02404	LiNi ₉ SnSr	12	-4.445	-4.711	1.500e-05	0.00621	0.655	1.524
snh_000_02405	Mn ₇ Sn ₈	15	-5.679	-5.961	-4.000e-06	0.00597	0.762	1.059
snh_000_02428	Al ₄ GaGeMn ₁₀ NdSb	18	-6.321	-6.659	0.000e+00	0.00448	0.476	0.982
snh_000_02435	Ge ₄ K ₂ Ru ₆ S	13	-5.639	-6.051	-2.000e-06	0.00677	1.373	1.241
snh_000_02499	Ni ₉ SbSn ₆ U	17	-4.924	-5.273	-7.000e-06	0.0075	1.071	2.049
snh_000_02595	Mn ₆ Sn ₇	13	-5.332	-5.895	-1.000e-06	0.0044	0.698	0.692
snh_000_02600	Al ₄ EuFe ₇	12	-5.611	-6.105	0.000e+00	0.00754	0.755	0.768
snh_000_02638	Cd ₂ Mn ₆ Se ₈ SrU	18	-5.26	-5.675	0.000e+00	0.00536	0.937	4.322
snh_000_02695	Cs ₅ Yb ₆	11	-0.819	-0.967	-2.200e-05	0.00167	2.346	3.933
snh_000_02701	Al ₂ Ni ₆ Si ₃ Yb ₃	14	-4.455	-4.706	5.000e-06	0.00701	0.617	0.566
snh_000_02776	Ru ₆ Sn ₇	13	-5.734	-6.111	-2.000e-06	0.00706	0.628	1.103
snh_000_02796	Ba ₂ Co ₆ Sn ₂	10	-5.038	-5.183	3.000e-06	0.00891	0.587	0.486
snh_000_02803	Cs ₄ Mn ₆ Sn ₂	12	-4.329	-4.809	-1.000e-06	0.00388	0.949	1.289
snh_000_02839	Ru ₇ Sn ₈	15	-5.856	-6.214	-2.000e-06	0.00481	0.734	0.626
snh_000_02886	BaRu ₆ Sn ₇	14	-5.399	-5.915	-1.000e-06	0.00544	0.371	0.484
snh_000_02887	Ru ₇ S ₅ TeTl	14	-6.196	-6.53	-5.000e-06	0.00386	0.803	1.515
snh_000_03010	I ₆ Ru ₆	12	-4.139	-5.019	-1.000e-05	0.00935	1.657	1.051
snh_000_03028	CaCdEuFe ₇ Sb ₅ Sn ₂	17	-4.95	-5.236	-1.100e-05	0.00983	1.258	1.638
snh_000_03048	AlNi ₆ Sn ₇	14	-4.479	-4.639	-1.000e-06	0.00985	1.379	1.185
snh_000_03087	Fe ₉ Na ₅ NiPSi ₃	19	-5.035	-5.409	-2.000e-05	0.00602	0.784	1.436
snh_000_03131	Mn ₇ Sn ₄	11	-6.184	-6.767	-2.000e-06	0.0055	0.823	0.899
snh_000_03135	Co ₆ Se ₆	12	-4.906	-5.452	0.000e+00	0.00414	0.67	0.867
snh_000_03157	Co ₆ Sn ₈	14	-4.872	-5.082	0.000e+00	0.00687	0.642	1.214
snh_000_03167	AlCo ₆ Pr ₂ Sn ₃	12	-5.364	-5.645	0.000e+00	0.00817	0.832	0.768
snh_000_03175	Al ₄ GeNi ₇	12	-4.589	-5.227	-1.100e-05	0.0054	1.453	1.582
snh_000_03224	Fe ₇ Te ₇	14	-4.869	-5.413	9.000e-06	0.00716	0.728	1.085
snh_000_03225	Fe ₇ Na ₃ Sn	11	-5.008	-5.388	-5.000e-06	0.00772	1.05	0.639
snh_000_03296	Nb ₂ Ru ₁₁ Si ₅	18	-8.104	-8.452	0.000e+00	0.00703	0.501	1.431
snh_000_03301	Ga ₃ NdRu ₈	12	-6.686	-7.263	-2.200e-05	0.00606	0.484	1.757
snh_000_03326	Fe ₆ Se ₆	12	-5.56	-5.981	-9.200e-05	0.00913	0.799	0.688
snh_000_03341	Al ₃ GdNi ₆ Pd ₃ Sr	14	-4.838	-5.044	0.000e+00	0.00956	0.49	0.95
snh_000_03370	Cs ₂ Ni ₈ Sn ₆	16	-3.981	-4.324	-1.000e-06	0.00877	0.996	2.53
snh_000_03409	Ni ₁₀ SbSnTb ₂	14	-5.05	-5.33	-2.000e-06	0.00482	0.817	0.824
snh_000_03464	Co ₆ Na ₂ Sn ₄	12	-4.484	-4.838	-5.000e-06	0.0073	1.068	0.714
snh_000_03479	Cs ₈ Yb ₆	14	-0.865	-0.952	-2.900e-05	0.00349	2.023	2.603
snh_000_03490	Na ₂ Ni ₈ Si ₂	12	-4.385	-4.843	-9.000e-06	0.00746	0.398	0.697
snh_000_03523	Co ₆ Sn ₈	14	-4.758	-5.111	-3.800e-05	0.00838	0.723	1.835
snh_000_03552	Co ₇ Ga ₃ K ₂ Li	13	-4.256	-4.433	1.000e-06	0.00532	0.684	0.512
snh_000_03653	CaMn ₆ Sn ₆	13	-5.573	-5.854	-7.000e-06	0.00778	0.707	1.637
snh_000_03673	Co ₆ LiSn ₆	13	-4.851	-5.086	-3.000e-06	0.00558	1.172	0.779
snh_000_03686	Co ₇ Sn ₃ Yb ₂	12	-4.901	-5.307	-5.000e-06	0.00616	0.412	1.024

Table S12. The profile of generated materials with Snub hexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
snh.000_03740	Fe ₆ Ga ₃ NiSr ₄	14	-4.65	-4.953	-5.000e-06	0.0075	1.2	0.84
snh.000_03769	Co ₆ Sr ₂ Tl	9	-4.6	-4.959	-8.000e-06	0.00507	1.005	0.739
snh_000_03784	Ni ₆ Sn ₆	12	-4.023	-4.7	-2.000e-05	0.0059	0.607	1.201
snh_000_03831	Cs ₅ Yb ₆	11	-0.852	-0.968	7.000e-06	0.00321	0.914	1.472
snh_000_03842	Cs ₆ Tb ₆	12	-1.968	-2.218	1.000e-06	0.00446	1.492	2.389
snh_000_03849	Ge ₂ Ni ₆ PrSn	10	-4.94	-5.356	-2.000e-06	0.00766	0.807	1.815
snh.000_03869	Al ₄ Ba ₂ Ru ₆	12	-5.844	-6.175	-3.000e-06	0.00316	0.828	0.602
snh_000_03873	Dy ₈ Ni ₇	15	-4.777	-5.21	-1.650e-04	0.00576	1.187	2.205
snh_000_03885	CdCs ₅ Yb ₆	12	-0.896	-0.992	-5.000e-06	0.00408	0.819	1.617
snh_000_03958	Ge ₃ MnRu ₉ Zr ₇	20	-8.116	-8.551	0.0000e+00	0.00671	1.086	1.165
snh_000_04071	Cs ₈ Yb ₆	14	-0.847	-0.952	-1.000e-06	0.0021	1.52	1.268
snh_000_04075	Ce ₂ Ga ₃ Ru ₉ Sb	15	-6.896	-7.32	-1.000e-05	0.00523	0.925	2.335
snh_000_04117	Cs ₆ Dy ₆	12	-1.825	-2.195	-4.400e-05	0.00906	1.356	2.223
snh_000_04126	Cs ₄ Yb ₆	10	-0.855	-0.982	-1.270e-04	0.00915	1.589	2.011
snh_000_04152	GeNi ₆ Pr ₂ Sn	10	-4.952	-5.352	0.0000e+00	0.00648	1.195	2.062
snh.000_04233	Fe ₆ La ₄ Sn ₄	14	-5.921	-6.158	5.000e-06	0.00671	0.565	0.48
snh_000_04278	Al ₇ Fe ₆ Pr	14	-5.426	-5.79	2.000e-05	0.00773	0.731	1.009
snh.000_04399	Eu ₂ PbRu ₉	12	-6.991	-7.338	-1.300e-05	0.00655	0.713	0.651
snh_000_04412	Al ₄ Fe ₆ Ge ₄ La ₄	18	-5.575	-5.86	0.0000e+00	0.00393	0.908	1.121
snh_000_04436	Ni ₆ SnTl ₄	11	-3.567	-3.979	3.000e-06	0.00355	1.121	1.545
snh_000_04459	Mn ₆ Sn ₇	13	-5.376	-5.884	-3.000e-06	0.00452	0.95	1.401
snh_000_04511	Cs ₅ Yb ₆	11	-0.866	-0.97	-1.000e-06	0.00169	0.981	3.157
snh_000_04530	Cs ₈ Tb ₆	14	-1.687	-2.014	1.000e-06	0.00255	1.723	3.005
snh_000_04541	Eu ₂ Ni ₇ Sn ₂	11	-4.395	-4.803	-1.150e-04	0.00954	0.863	2.006
snh_000_04542	Fe ₆ GaGeSb ₄	12	-5.508	-5.898	-3.100e-05	0.00591	0.954	1.882
snh_000_04547	Ge ₄ MgNi ₁₀	15	-4.923	-5.145	1.000e-06	0.00993	0.325	1.936
snh_000_04582	AgBrCo ₆ Sn ₅	13	-4.679	-4.893	-6.000e-06	0.00443	0.812	1.145
snh.000_04591	Mn ₆ SbSn ₇	14	-5.582	-5.819	-1.000e-06	0.00395	0.657	0.739
snh_000_04624	Ni ₉ Sn ₅	14	-4.66	-4.935	0.0000e+00	0.00926	0.737	1.472
snh_000_04627	BaRu ₈ Sn ₃	12	-6.579	-7.017	0.0000e+00	0.00993	0.692	1.236
snh.000_04636	GdNi ₆ SnTh	9	-5.379	-5.727	-1.300e-05	0.00865	0.457	0.45
snh.000_04663	Mn ₇ Sn ₇	14	-5.634	-6.135	-1.200e-05	0.00593	0.866	0.944
snh.000_04786	Mn ₆ Rb ₂ Se ₄	12	-5.46	-5.945	-2.000e-06	0.00824	1.05	0.807
snh_000_04819	Al ₇ Co ₆	13	-5.052	-5.658	-1.100e-05	0.00682	1.272	2.287
snh_000_04820	Fe ₆ Se ₅ Te ₂	13	-5.244	-5.692	9.000e-06	0.00968	0.703	1.164
snh_000_04836	Ba ₂ Mn ₈ PSiSn ₄	16	-5.888	-6.227	-4.000e-06	0.00595	0.896	1.627
snh.000_04856	Ru ₆ Sn ₈	14	-5.697	-6.033	3.000e-06	0.00441	0.363	0.439
snh_000_04937	Co ₃ Mn ₇ SiSn ₉	20	-5.244	-5.984	-2.000e-05	0.00806	1.03	2.408
snh_000_04942	FeMn ₆ Si ₆ Zr ₃	16	-7.468	-7.799	-1.000e-05	0.00944	0.572	1.302
snh_000_04954	Mn ₇ Sn ₅	12	-6.017	-6.454	-1.000e-06	0.0066	1.108	2.038
snh_000_04978	Co ₇ Sn ₃ Tl ₂	12	-4.809	-5.063	2.000e-06	0.00655	0.655	1.115
snh_001_00172	Cs ₈ Yb ₆	14	-0.839	-0.952	2.000e-06	0.00366	1.168	2.679
snh_001_00178	Ru ₆ Sn ₈	14	-5.776	-6.037	-7.000e-06	0.00627	0.478	0.674
snh_001_00184	Cs ₄ Dy ₆	10	-2.273	-2.421	-6.000e-06	0.00415	0.665	2.631
snh_001_00218	Fe ₆ Se ₆	12	-5.526	-5.981	-5.000e-05	0.00777	1.003	0.754
snh_001_00231	Mn ₆ Sn ₇	13	-5.396	-5.873	3.000e-06	0.00554	1.053	1.47
snh_001_00278	Cs ₈ Dy ₆	14	-1.702	-1.998	-3.000e-06	0.00381	1.972	1.556
snh.001_00292	Ca ₂ Ge ₅ Ru ₈ U	16	-6.748	-7.072	0.0000e+00	0.00778	0.429	0.915
snh_001_00311	AlCaEuNi ₆ Sn	10	-4.495	-4.728	-1.000e-06	0.00457	0.938	1.105
snh_001_00316	Ru ₆ Sn ₆	12	-5.563	-6.329	-5.000e-06	0.00932	0.79	1.326
snh.001_00319	Pd ₈ Ru ₇ Sm	16	-6.296	-6.805	0.0000e+00	0.00481	0.518	0.601
snh_001_00355	Ba ₂ Co ₈ Ge ₆ Sn ₂	18	-4.899	-5.351	1.000e-06	0.00702	0.885	1.415

Table S12. The profile of generated materials with Snub hexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
snh_001_00362	Au ₂ Fe ₉ Sn ₅	16	-5.539	-5.895	1.000e-06	0.00657	0.6	0.617
snh_001_00413	Co ₆ Sn ₆ Y ₂	14	-5.389	-5.731	-1.400e-05	0.00702	0.232	1.075
snh_001_00450	Cs ₂ Ga ₅ Ru ₆	13	-5.056	-5.298	1.000e-06	0.00435	0.535	0.88
snh_001_00516	BaGa ₆ Mn ₇	14	-5.394	-5.77	-2.000e-06	0.0065	0.373	1.132
snh_001_00564	Cs ₆ Yb ₆	12	-0.844	-0.96	-7.200e-05	0.00351	2.437	2.604
snh_001_00599	Ce ₄ Ru ₆	10	-7.539	-8.258	-3.600e-05	0.00562	1.483	1.199
snh_001_00646	Cs ₄ Dy ₆ SbSn	12	-2.865	-3.02	-2.400e-05	0.0073	0.882	0.618
snh_001_00702	BaGa ₂ Ni ₇ Sn ₃ Zn	14	-3.858	-4.367	-2.200e-05	0.00879	0.52	0.762
snh_001_00824	AlNi ₇ Sn ₅	13	-4.463	-4.854	-1.000e-06	0.00855	0.296	1.834
snh_001_00855	Ni ₇ Sn ₆ Sr ₂	15	-4.38	-4.555	0.000e+00	0.00817	0.197	0.602
snh_001_00856	Al ₃ Ba ₂ Mn ₆ Sb	12	-5.54	-5.94	-1.000e-06	0.00646	0.471	0.625
snh_001_00875	Cs ₄ Mn ₆ Sn ₂	12	-4.397	-4.957	-8.000e-06	0.00294	1.304	1.775
snh_001_00909	GeNi ₈ Sn ₃	12	-4.803	-5.069	2.000e-06	0.00922	1.039	0.726
snh_001_00921	Al ₆ Mn ₇ Sb	14	-5.798	-6.4	-5.200e-05	0.00363	0.584	1.299
snh_001_00936	Cs ₃ Ru ₆ Sn	10	-5.178	-5.544	0.000e+00	0.00635	0.745	1.347
snh_001_00938	Rb ₅ Ru ₆ Sn ₃	14	-4.346	-4.711	1.000e-06	0.00781	0.756	1.235
snh_001_01005	Mn ₆ Sn ₄ Sr ₄	14	-5.143	-5.369	0.000e+00	0.00672	0.506	1.125
snh_001_01014	Cs ₆ Yb ₆	12	-0.807	-0.96	0.000e+00	0.00238	1.693	3.213
snh_001_01025	Cs ₆ Yb ₆	12	-0.807	-0.936	-1.000e-06	0.00244	1.188	3.24
snh_001_01059	Ru ₇ Se ₇	14	-5.929	-6.368	-1.000e-06	0.00773	0.984	0.781
snh_001_01105	Mn ₆ Pr ₃ SbSn ₅	15	-5.777	-6.162	-4.000e-06	0.00506	0.957	1.659
snh_001_01140	Ni ₇ Sn ₇	14	-4.399	-4.756	-1.100e-05	0.0072	0.822	1.453
snh_001_01200	BaCo ₇ Sn ₆	14	-4.881	-5.191	2.000e-06	0.00479	0.834	1.753
snh_001_01223	Co ₁₁ Ge ₄ La	16	-6.024	-6.278	0.000e+00	0.00717	0.329	0.449
snh_001_01267	Co ₇ Na ₄	11	-4.202	-4.43	3.000e-06	0.0091	0.65	0.529
snh_001_01307	Ga ₃ Ge ₄ Ni ₁₃	20	-5.038	-5.118	0.000e+00	0.00828	0.311	0.315
snh_001_01314	Co ₁₀ Pr ₂	12	-6.106	-6.428	-1.300e-05	0.00548	0.705	1.132
snh_001_01368	Al ₆ Dy ₂ Fe ₆	14	-5.421	-5.881	-1.470e-04	0.00997	1.037	0.94
snh_001_01460	Al ₃ BaGe ₂ Ni ₇	13	-4.665	-4.918	-1.000e-06	0.00984	0.497	1.345
snh_001_01484	AlCo ₉ GaNdSnYb	14	-5.253	-5.691	-2.000e-06	0.00479	0.759	0.741
snh_001_01489	Ca ₂ Co ₇ PY ₅	15	-5.903	-6.17	1.800e-05	0.00705	0.634	1.309
snh_001_01514	Cs ₆ Nd ₆	12	-2.068	-2.349	-7.000e-06	0.00285	1.738	1.638
snh_001_01528	Cs ₅ Nd ₆	11	-2.12	-2.466	2.000e-06	0.00213	1.259	2.562
snh_001_01578	Al ₂ CeErRu ₉ ScSi ₅	19	-6.942	-7.391	0.000e+00	0.0067	0.438	1.983
snh_001_01604	BaNa ₅ Ni ₇ Sn ₂	15	-3.219	-3.581	2.000e-06	0.00671	0.542	1.261
snh_001_01615	Cs ₂ Ru ₆ Se ₄	12	-5.483	-6.02	0.000e+00	0.00543	1.512	1.061
snh_001_01627	Al ₂ EuNi ₇ Si ₂	12	-4.933	-5.265	3.000e-06	0.00735	1.009	0.823
snh_001_01675	Ge ₇ Ru ₁₀ Sn ₂	19	-6.502	-6.937	0.000e+00	0.00654	0.718	1.422
snh_001_01682	La ₂ Ni ₁₀	12	-5.197	-5.485	-5.000e-06	0.00771	0.581	0.508
snh_001_01693	Co ₉ Lu ₃ SiY	14	-6.069	-6.439	-3.500e-05	0.00843	1.233	1.58
snh_001_01773	Ni ₆ Sn ₈	14	-4.498	-4.632	-3.000e-06	0.00927	0.461	0.674
snh_001_01814	Mn ₆ Sn ₆	12	-5.771	-6.144	-3.200e-05	0.00606	1.085	1.883
snh_001_01832	Br ₆ Ru ₆	12	-4.585	-5.207	-4.000e-06	0.00441	1.347	1.938
snh_001_01839	Ru ₆ Sn ₄ Tl ₂	12	-5.694	-6.048	-9.000e-06	0.00683	0.84	0.737
snh_001_01896	AlGe ₂ La ₂ Ru ₇ Zr ₄	16	-7.319	-7.779	0.000e+00	0.00922	0.365	1.181
snh_001_01905	Co ₆ Sn ₂ Sr ₂	10	-4.703	-5.142	-3.800e-05	0.00531	0.415	1.668
snh_001_01916	Ru ₆ Sn ₈	14	-5.402	-5.992	0.000e+00	0.00947	0.445	0.759
snh_001_02020	Ni ₆ Se ₄ Tl ₂	12	-4.021	-4.443	1.000e-06	0.00652	2.24	1.476
snh_001_02031	Co ₆ Sn ₂ Tl ₂	10	-4.644	-5.088	1.000e-06	0.00853	0.853	2.193
snh_001_02134	Ce ₂ Ru ₉ Sn	12	-7.776	-8.16	3.000e-06	0.00829	0.396	1.402
snh_001_02197	AlNa ₃ Ni ₇ Sn ₂	13	-3.829	-4.102	-3.600e-05	0.00977	1.022	1.638
snh_001_02206	Cs ₅ PbYb ₆	12	-1.181	-1.266	-1.000e-06	0.00325	0.95	3.136

Table S12. The profile of generated materials with Snub hexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
snh_001_02285	Ga ₃ LiMn ₆ Sn ₂ Sr ₄	16	-4.244	-4.837	-2.000e-06	0.00629	1.59	2.178
snh_001_02330	Co ₁₂ Na ₂	14	-5.257	-5.608	8.000e-06	0.00854	0.656	1.22
snh_001_02401	Co ₆ Tl ₆	12	-3.973	-4.197	-3.900e-05	0.00726	0.799	1.339
snh_001_02404	Ni ₆ Zr ₈	14	-7.233	-7.47	0.000e+00	0.00847	0.474	1.531
snh_001_02445	Ru ₆ SeTe ₃ Tl ₂	12	-5.267	-5.813	1.000e-06	0.00589	1.031	1.786
snh_001_02464	Ba ₂ Mn ₆ Se ₅	13	-5.684	-6.095	-2.000e-06	0.00598	0.761	1.274
snh_001_02465	Ru ₆ Sn ₈	14	-5.824	-6.001	-2.000e-06	0.00817	0.649	1.478
snh_001_02472	Ni ₆ Sn ₃ Sr ₅	14	-3.712	-3.985	-5.000e-06	0.00634	0.902	1.778
snh_001_02482	Cs ₄ Yb ₆	10	-0.882	-0.983	-1.110e-05	0.00148	1.794	1.409
snh_001_02493	Cl ₆ Mn ₆	12	-5.017	-5.566	-9.000e-06	0.00937	0.821	1.544
snh_001_02539	Al ₅ ErFe ₈ Ge ₂ Sn ₄	20	-5.311	-5.606	-1.000e-05	0.00686	0.647	1.291
snh_001_02664	Co ₆ Sn ₈	14	-4.856	-5.112	2.000e-06	0.00711	0.86	1.338
snh_001_02706	Fe ₆ Ga ₃ Nd ₄ Te	14	-5.401	-5.805	-7.000e-06	0.00446	0.781	0.926
snh_001_02813	Fe ₆ La ₂ Sn ₆	14	-5.266	-5.866	1.000e-06	0.00445	1.066	0.868
snh_001_02825	Co ₈ EuGe ₃ SnY	14	-5.75	-5.985	1.000e-06	0.00744	0.511	1.257
snh_001_02839	Ni ₆ Sn ₈	14	-4.287	-4.626	1.000e-06	0.00767	1.028	1.02
snh_001_02856	Al ₅ Ru ₆ TlYb ₂	14	-5.204	-5.812	-5.000e-06	0.00432	0.942	1.875
snh_001_02866	Co ₆ Se ₄ Tl ₂	12	-4.71	-5.01	-2.000e-06	0.00918	0.658	1.167
snh_001_02908	Ba ₂ Ni ₇ Sn ₄	13	-4.128	-4.565	-5.000e-06	0.00892	0.766	0.924
snh_001_03041	AgLi ₂ Ni ₆ Sn ₃	12	-3.919	-4.295	-4.000e-06	0.00557	0.782	0.733
snh_001_03050	Mn ₇ Sn ₈	15	-5.534	-5.965	-1.000e-06	0.00513	0.771	1.792
snh_001_03067	Ga ₈ Ru ₆ Te ₂	16	-5.049	-5.369	-2.700e-05	0.00987	0.674	2.344
snh_001_03106	Ni ₆ Sn ₆	12	-4.431	-4.795	-1.200e-05	0.00661	0.39	1.176
snh_001_03124	Br ₆ Mn ₆	12	-4.37	-5.19	-1.400e-05	0.00631	1.058	2.241
snh_001_03185	Co ₆ Se ₆	12	-4.977	-5.441	-1.600e-05	0.00773	0.848	2.655
snh_001_03216	BrGeMn ₆ Sn ₄	12	-5.498	-5.926	-2.000e-06	0.00803	1.009	1.182
snh_001_03360	Co ₆ La ₆ LiPb ₂	15	-5.336	-5.475	0.000e+00	0.00988	0.402	0.578
snh_001_03380	Ge ₄ Ru ₉ Zr ₅	18	-7.726	-8.265	0.000e+00	0.00656	0.802	1.133
snh_001_03383	La ₂ Ni ₁₀	12	-5.219	-5.483	-1.000e-06	0.0074	0.492	0.44
snh_001_03438	Cs ₅ KNd ₆	12	-2.042	-2.368	-5.000e-06	0.0038	1.751	2.102
snh_001_03515	Rb ₂ Ru ₆ Sn ₄	12	-5.46	-5.734	-7.000e-06	0.0053	0.48	1.576
snh_001_03544	Mn ₆ S ₆	12	-6.401	-6.91	0.000e+00	0.00587	0.618	0.66
snh_001_03556	Al ₆ Fe ₆ Sr ₂	14	-5.04	-5.299	2.000e-06	0.00574	0.596	0.703
snh_001_03589	Al ₄ Mn ₆ Tl ₄	14	-4.79	-5.217	-9.000e-06	0.00969	1.256	1.591
snh_001_03625	Co ₇ Ga ₆ Y ₂	15	-5.274	-5.503	1.000e-06	0.00703	0.995	1.352
snh_001_03628	Ni ₆ Sn ₅ Sr ₃	14	-4.081	-4.369	0.000e+00	0.00746	1.068	1.944
snh_001_03659	Mn ₆ Sn ₆	12	-5.776	-6.142	1.000e-06	0.00492	0.964	1.873
snh_001_03662	Br ₃ Cl ₃ Ru ₆	12	-4.783	-5.304	-1.800e-05	0.00628	1.119	1.417
snh_001_03760	Ce ₃ Ru ₈ SiSn ₂	14	-7.011	-7.638	0.000e+00	0.00907	0.828	2.816
snh_001_03785	DyNi ₁₂ Sr	14	-4.859	-5.132	-1.900e-05	0.008	0.573	1.723
snh_001_03843	Al ₂ La ₄ Ni ₆ SiSn	14	-5.249	-5.376	9.000e-06	0.00906	0.415	0.631
snh_001_03959	KMn ₆ Se ₃ SnTl	12	-5.38	-5.962	-6.000e-06	0.00625	0.975	1.296
snh_001_03971	Ge ₃ La ₄ Ni ₆ Sn	14	-5.323	-5.526	-2.000e-06	0.00845	1.156	1.934
snh_001_04001	Fe ₆ LaSbSn ₄ Sr ₂	14	-5.278	-5.517	-6.000e-06	0.00981	0.846	3.08
snh_001_04013	AlCeCo ₆ Nd ₂	10	-5.913	-6.307	-5.000e-06	0.00666	0.844	0.548
snh_001_04107	Ni ₆ Sn ₄ Sr ₄	14	-3.745	-4.221	-1.500e-05	0.00731	0.832	1.224
snh_001_04112	Co ₆ La ₇ Sn	14	-5.666	-5.831	0.000e+00	0.00884	0.375	0.855
snh_001_04141	Ni ₉ SbSn ₂	12	-4.818	-5.119	0.000e+00	0.00978	0.461	3.352
snh_001_04143	Mn ₆ Sn ₉	15	-4.979	-5.655	-5.000e-06	0.00891	0.748	1.95
snh_001_04154	Ni ₆ Sn ₈	14	-4.419	-4.628	0.000e+00	0.00843	0.563	0.966
snh_001_04216	Ni ₆ Sn ₈	14	-4.435	-4.629	-3.000e-06	0.00787	0.53	0.777
snh_001_04217	Ca ₈ Ni ₆	14	-3.361	-3.547	-5.000e-06	0.00819	1.073	1.091

Table S12. The profile of generated materials with Snub hexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
snh_001_04218	Mn ₆ Sn ₆	12	-5.384	-6.126	2.000e-06	0.00698	1.1	0.93
snh_001_04219	Ge ₂ Ni ₇ Sn ₃	12	-4.618	-5.022	-2.000e-06	0.00499	0.37	1.26
snh_001_04257	CaGaNi ₇ Sn ₃	12	-4.237	-4.754	2.000e-06	0.00501	0.289	0.73
snh_001_04275	Ni ₈ Pr ₂ Sn ₅	15	-4.871	-5.058	-2.000e-06	0.00484	0.773	1.394
snh_001_04315	Ni ₆ Sn ₆	12	-4.536	-4.714	-2.000e-06	0.00962	0.647	0.669
snh_001_04337	AlNi ₇ Sn ₃	11	-4.645	-5.074	-1.000e-06	0.00648	1.02	1.988
snh_001_04413	AlAsGa ₂ La ₃ Ni ₆ Sn	14	-4.859	-5.106	6.000e-06	0.0066	1.198	1.141
snh_001_04506	Co ₆ Te ₆	12	-4.789	-5.115	-2.000e-06	0.00924	0.743	0.715
snh_001_04507	Cs ₆ Tb ₆	12	-1.825	-2.287	-4.000e-05	0.00651	2.175	4.033
snh_001_04513	Cs ₅ Yb ₇	12	-0.861	-0.991	4.300e-05	0.00856	0.598	1.903
snh_001_04571	Cl ₆ Mn ₆	12	-4.924	-5.464	-1.000e-06	0.00743	0.647	1.399
snh_001_04598	Co ₆ Rb ₃ Sn ₅	14	-4.249	-4.477	-4.000e-06	0.00808	1.259	2.124
snh_001_04632	BaNi ₇ Sn ₄	12	-4.39	-4.729	-3.800e-05	0.008	0.914	1.681
snh_001_04704	Ni ₆ Te ₆	12	-4.145	-4.473	-9.000e-06	0.0054	0.618	1.631
snh_001_04765	Co ₇ Se ₄ Sn ₅	16	-4.855	-5.108	1.000e-06	0.00891	0.345	1.152
snh_001_04872	GeMn ₆ Pd ₄ Sn ₂	13	-5.941	-6.539	-2.000e-06	0.00818	0.72	2.485
snh_001_04946	Ni ₆ Se ₆ Tl ₂	14	-4.034	-4.357	-1.100e-05	0.00777	1.093	1.806
snh_001_04959	Co ₇ EuGeSn ₃	12	-5.021	-5.527	1.000e-06	0.00637	0.877	2.144
snh_001_05028	I ₆ Ru ₆	12	-4.803	-4.994	-2.000e-06	0.00943	0.514	0.616
snh_001_05122	Fe ₆ Ge ₃ La ₂ Rh	12	-6.408	-6.726	7.000e-06	0.00611	0.584	1.011
snh_002_00012	BaNi ₆ Se ₇	14	-4.322	-4.708	-1.020e-04	0.00619	0.591	0.657
snh_002_00049	Cs ₈ Dy ₆	14	-1.684	-2.0	-4.000e-06	0.00183	2.204	1.614
snh_002_00050	Ba ₂ PrRu ₉ Sn ₄	16	-6.337	-6.658	0.000e+00	0.00674	0.568	0.727
snh_002_00074	Fe ₆ La ₈	14	-6.028	-6.19	-4.000e-06	0.00882	0.617	0.791
snh_002_00089	Ru ₁₂ Sn ₆ Tb ₂	20	-6.773	-7.081	0.000e+00	0.00362	0.588	0.928
snh_002_00101	BaGe ₄ MgRu ₆ Sr ₂	14	-5.576	-5.831	1.000e-06	0.00627	0.306	0.55
snh_002_00187	Ge ₈ Mn ₆	14	-5.966	-6.323	-4.000e-06	0.00536	0.17	0.984
snh_002_00280	Rb ₂ Ru ₆ Sn ₄	12	-5.451	-5.735	-5.000e-06	0.00782	0.515	1.572
snh_002_00327	LaRu ₆ Tl ₇	14	-4.79	-5.139	0.000e+00	0.00639	0.902	0.905
snh_002_00339	Cs ₅ Tb ₆	11	-2.179	-2.306	-4.000e-06	0.00364	0.729	2.201
snh_002_00389	Ru ₆ SbSn ₇	14	-5.724	-6.081	3.000e-06	0.00687	0.642	1.167
snh_002_00451	Al ₃ Co ₆ Yb ₅	14	-4.253	-4.414	9.000e-06	0.00866	0.212	0.35
snh_002_00533	Ge ₅ Mn ₆ RuSn ₃	15	-5.972	-6.331	4.000e-06	0.00491	0.694	0.661
snh_002_00535	NdNi ₈ Sn ₇	16	-4.756	-4.903	2.000e-06	0.00802	0.297	0.58
snh_002_00540	Fe ₁₁ Ge ₅ Ho	17	-6.489	-6.85	0.000e+00	0.00689	0.386	0.758
snh_002_00624	Co ₆ Li ₅ Sn ₃	14	-4.241	-4.43	3.000e-06	0.00661	0.758	0.668
snh_002_00626	Co ₇ Ge ₃ PrSe ₂	13	-5.432	-5.809	0.000e+00	0.00574	1.195	2.319
snh_002_00629	Ni ₇ Sn ₆	13	-4.657	-4.787	0.000e+00	0.0092	1.131	1.047
snh_002_00652	Br ₆ Ru ₆	12	-4.367	-5.204	-5.000e-06	0.00706	1.465	1.821
snh_002_00679	AlErFe ₆ Ge ₂ Sb ₂ Si ₂	14	-5.672	-6.132	-8.000e-06	0.00512	0.844	1.296
snh_002_00716	Al ₂ Ru ₁₆ Sb	19	-7.876	-8.188	1.000e-05	0.00553	0.359	0.449
snh_002_00740	BaLaNdPdRu ₈ Sn	13	-6.862	-7.131	2.000e-06	0.0061	0.819	0.824
snh_002_00816	Ge ₄ Ru ₆ S ₂ Sr ₂	14	-5.86	-6.261	1.000e-06	0.00476	0.812	1.105
snh_002_00891	Al ₈ LiMn ₆	15	-5.306	-5.701	-1.000e-06	0.00874	0.848	0.584
snh_002_00900	Mn ₆ Sn ₇	13	-5.643	-5.897	1.000e-06	0.00665	0.622	1.227
snh_002_00910	Eu ₂ Ni ₇ Sn ₅	14	-4.397	-4.695	-5.000e-06	0.00671	0.986	0.86
snh_002_01139	Cs ₅ Yb ₆	11	-0.906	-0.968	-4.000e-06	0.00177	0.575	1.546
snh_002_01155	CaCdRu ₇ Sn ₄ Yb	14	-5.582	-5.916	1.900e-05	0.0089	0.511	0.718
snh_002_01169	NaNi ₇ Sn ₃	11	-4.359	-4.664	1.000e-06	0.00727	1.188	1.895
snh_002_01185	Cs ₂ Ni ₆ Te ₄	12	-3.91	-4.131	1.500e-05	0.00873	0.967	1.259
snh_002_01218	Cs ₈ Nd ₆	14	-2.044	-2.136	-1.000e-06	0.00313	1.13	1.916
snh_002_01266	Co ₁₂ Ge ₃ Ti ₂	17	-6.471	-6.729	0.000e+00	0.00961	0.363	0.823

Table S12. The profile of generated materials with Snub hexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
snh_002_01339	LiNdNi ₆ Sn ₂	10	-4.517	-4.889	1.000e-06	0.00889	0.871	2.321
snh_002_01452	Ru ₆ Sn ₁₂	18	-4.369	-5.532	-1.500e-05	0.00997	1.099	1.33
snh_002_01478	Ni ₉ Sn ₅	14	-4.721	-5.026	-8.000e-06	0.00574	0.782	2.083
snh_002_01564	Ru ₆ Sn ₈	14	-5.838	-6.021	-3.000e-06	0.00502	0.319	0.461
snh_002_01657	Ni ₆ Tl ₆	12	-3.502	-3.649	-6.000e-06	0.00427	0.45	0.489
snh_002_01692	ClGeMn ₆ NaTe ₅	14	-5.083	-5.527	3.000e-06	0.0064	0.685	1.839
snh_002_01702	Ni ₆ SSn ₄	11	-4.516	-4.858	-2.200e-05	0.00573	0.624	1.896
snh_002_01727	Ni ₇ Sn ₆ Tb	14	-4.631	-4.922	0.000e+00	0.0077	0.371	1.11
snh_002_01782	Cs ₅ Yb ₈	13	-0.864	-1.003	-1.000e-06	0.00215	0.82	1.088
snh_002_01813	Mn ₆ Sn ₆	12	-5.761	-6.142	-2.600e-05	0.00822	0.981	1.418
snh_002_01902	Ge ₂ PRu ₇ Sn ₄	14	-6.19	-6.665	0.000e+00	0.00475	1.035	1.307
snh_002_01985	Na ₃ Ni ₈	11	-3.762	-4.094	-1.100e-05	0.00804	0.391	0.569
snh_002_01993	Al ₃ Hf ₃ Ru ₆ SbSn	14	-7.292	-7.721	0.000e+00	0.00663	0.558	0.904
snh_002_02029	AlCo ₈ La ₂ PrSi	13	-5.917	-6.222	-1.000e-06	0.00894	0.563	1.715
snh_002_02069	Ge ₂ Mn ₆ Sn ₆	14	-5.648	-5.904	-2.000e-06	0.00675	0.537	1.013
snh_002_02077	Mn ₇ Sn ₃ Zn	11	-6.133	-6.534	-7.000e-06	0.00661	0.873	1.886
snh_002_02130	Co ₆ Sr ₃	9	-4.52	-4.898	-1.000e-06	0.00825	1.022	1.395
snh_002_02168	Cs ₅ GeYb ₆	12	-1.081	-1.35	-1.000e-06	0.00282	1.354	2.538
snh_002_02171	GeNdRu ₈ Sn ₇	17	-6.086	-6.441	-1.000e-05	0.00912	0.838	1.589
snh_002_02218	Cs ₈ Nd ₆	14	-1.869	-2.137	1.000e-06	0.00311	1.678	2.178
snh_002_02223	Ba ₂ Ni ₆ Se ₅	13	-4.438	-4.726	-1.000e-06	0.00749	1.071	1.667
snh_002_02238	Co ₆ Sn ₈	14	-4.9	-5.076	0.000e+00	0.00738	0.609	0.598
snh_002_02259	Ge ₅ Ni ₁₀ Tb	16	-5.102	-5.379	-6.500e-05	0.00562	0.258	1.108
snh_002_02346	Eu ₄ Ru ₆ Sn ₅	15	-5.295	-5.66	-2.000e-06	0.00566	1.003	1.144
snh_002_02425	Co ₈ Nd ₂ Sn	11	-5.74	-6.258	-2.200e-05	0.00604	1.253	2.383
snh_002_02437	Ba ₂ Co ₆ Ga ₄	12	-4.604	-4.762	-2.000e-06	0.00493	0.38	0.871
snh_002_02502	Al ₆ Mn ₆ Ni ₂	14	-5.765	-6.346	-1.900e-05	0.00516	0.641	1.04
snh_002_02556	Mn ₆ SSb ₆ Sn	14	-5.779	-6.109	-1.000e-06	0.00577	0.657	0.865
snh_002_02564	Cs ₂ Ru ₆ SnTe ₂	11	-5.245	-5.848	-5.000e-06	0.00566	0.995	0.844
snh_002_02575	BaCo ₆ La ₂ NdSn ₂	12	-5.404	-5.667	-4.000e-06	0.00484	0.823	0.945
snh_002_02654	Fe ₇ Zr ₈	15	-7.929	-8.422	-5.000e-05	0.00628	0.576	1.638
snh_002_02733	Ag ₂ Ba ₂ GeNi ₆	11	-4.024	-4.198	-6.000e-06	0.00629	0.617	0.49
snh_002_02791	Cd ₂ Ru ₆ Sr ₂	10	-5.286	-5.693	-2.000e-06	0.00472	0.467	0.589
snh_002_02888	Fe ₇ LaSn ₆	14	-5.692	-5.907	-8.000e-06	0.00894	0.656	0.797
snh_002_02925	Co ₇ NdSn ₃	11	-5.513	-5.874	-1.000e-05	0.00451	0.433	0.542
snh_002_02926	Ru ₆ Sn ₈	14	-5.567	-6.011	0.000e+00	0.00603	0.505	0.615
snh_002_02969	Co ₉ NdSn ₉	19	-5.152	-5.362	-1.000e-05	0.00813	0.318	1.544
snh_002_02980	Co ₆ La ₂ Pr	9	-5.745	-6.32	-2.500e-05	0.00849	0.565	0.523
snh_002_02991	Cs ₂ Ru ₆ S ₃ Se	12	-5.521	-6.145	-1.000e-06	0.00607	1.421	1.563
snh_002_03040	Al ₂ Co ₆ Eu ₂	10	-4.985	-5.429	-4.000e-06	0.00869	0.792	1.136
snh_002_03114	Ni ₁₁ Sn ₅ Yb	17	-4.686	-4.905	-9.000e-06	0.00888	0.677	0.649
snh_002_03262	Co ₆ Sn ₈	14	-4.697	-5.069	-2.000e-06	0.00731	0.796	0.881
snh_002_03264	GeMn ₆ SSn ₄ Sr	13	-5.737	-6.046	0.000e+00	0.00411	0.752	1.974
snh_002_03275	Nd ₃ Ni ₉ Sn ₂	14	-5.049	-5.366	1.000e-06	0.00806	0.873	1.158
snh_002_03295	Ni ₆ Sn ₆	12	-4.405	-4.792	-2.000e-06	0.00587	0.49	1.192
snh_002_03317	Br ₆ Mn ₆	12	-4.614	-5.195	0.000e+00	0.00865	1.009	1.112
snh_002_03378	Ni ₈ Sn ₈	16	-4.441	-4.737	1.000e-06	0.00698	1.085	1.026
snh_002_03386	Cs ₈ Yb ₆	14	-0.807	-0.949	-2.000e-06	0.00214	1.74	2.497
snh_002_03408	Ni ₈ Sn ₈	16	-4.371	-4.727	-1.000e-06	0.00511	0.789	0.912
snh_002_03448	Co ₂ Li ₄ Mn ₇ Sb ₂ Se ₅	20	-5.209	-5.677	0.000e+00	0.00952	0.464	2.455
snh_002_03472	Ge ₂ Ni ₇ PrSn	11	-5.011	-5.281	0.000e+00	0.00665	0.863	0.571
snh_002_03519	CeMn ₈ NiSn ₄	14	-6.057	-6.849	-4.000e-06	0.00526	0.951	1.858

Table S12. The profile of generated materials with Snub hexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
snh_002_03621	Co ₆ Nd ₂ Sn	9	-5.588	-6.137	-5.000e-06	0.00591	1.431	1.3
snh_002_03654	Ce ₃ NbRu ₁₀ SbSi ₃	18	-7.734	-8.081	0.000e+00	0.0053	0.509	1.337
snh_002_03661	AuCdHf ₂ Mn ₇ RuSi ₂ Sn	15	-6.92	-7.308	0.000e+00	0.00698	0.657	1.082
snh_002_03697	GeNi ₆ Sn ₂ Tl ₂	11	-4.26	-4.486	-1.900e-05	0.00555	0.585	1.397
snh_002_03715	Mn ₁₀ Nb ₂ NdSi ₆	19	-7.561	-7.944	-2.000e-05	0.00623	0.724	0.994
snh_002_03758	CdCo ₆ Ga ₄ Zr ₃	14	-5.571	-5.888	2.000e-06	0.00537	0.57	0.578
snh_002_03781	Ni ₆ Sn ₈	14	-4.44	-4.629	3.000e-06	0.00835	0.512	0.694
snh_002_03840	Cs ₂ Ru ₆ Se ₄	12	-5.521	-5.96	-1.100e-05	0.00601	1.275	1.0
snh_002_03894	Br ₆ Cl ₄ CoLiRu ₆ SeTe	20	-3.775	-4.407	-3.000e-06	0.0084	1.53	1.822
snh_002_03895	Mn ₇ SnTl ₂	10	-5.719	-6.612	1.000e-06	0.00582	1.41	0.887
snh_002_03901	Al ₃ Ga ₂ NaNi ₆ Sn ₃	15	-3.994	-4.411	-5.000e-06	0.00734	0.97	2.25
snh_002_03964	I ₄ Ru ₆ S	11	-4.654	-5.624	-1.000e-06	0.0077	2.175	2.558
snh_002_03971	Al ₂ NdNi ₉ Pr ₃ Si	16	-5.161	-5.361	-1.730e-04	0.00821	0.552	1.779
snh_002_04029	Fe ₇ Ga ₇ Sr	15	-4.875	-5.282	-6.000e-06	0.00682	0.552	1.097
snh_002_04117	Ni ₆ Sn ₆	12	-4.418	-4.703	-4.000e-06	0.00765	0.623	0.775
snh_002_04188	BaRu ₆ Sn ₆ Yb	14	-5.607	-5.859	-4.000e-06	0.00656	0.556	1.014
snh_002_04242	As ₆ BiFe ₇	14	-5.95	-6.251	4.000e-06	0.00943	0.575	0.628
snh_002_04376	Co ₆ Ge ₃ Sr ₂	11	-5.056	-5.339	7.000e-06	0.00556	0.556	0.99
snh_002_04384	Co ₆ LaSbSn ₂	10	-5.339	-5.886	5.000e-06	0.00751	0.641	0.848
snh_002_04396	La ₄ Ni ₆ Sn ₄	14	-5.153	-5.317	-2.000e-06	0.0077	0.71	1.043
snh_002_04406	BiNi ₉ Sn ₂	12	-4.749	-5.007	2.000e-06	0.00423	0.863	1.142
snh_002_04451	GeMn ₆ PbScSn ₅	14	-5.472	-6.062	-1.000e-06	0.00581	0.634	0.889
snh_002_04466	Mn ₉ Sn ₇	16	-6.042	-6.429	-1.000e-05	0.00643	0.687	1.153
snh_002_04491	Cs ₃ Ni ₆ Sn ₃	12	-3.729	-3.886	-1.000e-06	0.00607	0.605	0.727
snh_002_04501	CaMn ₆ Sn ₇	14	-5.343	-5.735	1.000e-06	0.00748	0.742	1.238
snh_002_04611	Cs ₂ Ga ₄ Ru ₆	12	-5.099	-5.354	2.000e-06	0.00516	1.114	1.377
snh_002_04662	Ga ₈ La ₂ Mn ₆	16	-5.265	-5.522	0.000e+00	0.00267	0.568	1.085
snh_002_04667	Al ₂ Ge ₇ Ru ₆ SiSn ₃	19	-5.169	-5.875	-3.000e-05	0.00793	1.082	1.469
snh_002_04709	Co ₁₂ Sn ₃ U ₂	17	-6.641	-6.903	-2.000e-05	0.00725	0.595	1.415
snh_002_04755	AlBaEuGa ₃ Ru ₇	13	-5.967	-6.245	-3.000e-06	0.00732	0.32	0.547
snh_002_04782	Ge ₂ Ni ₆ Tl ₃	11	-4.003	-4.333	-4.000e-06	0.00914	0.797	1.293
snh_002_04788	Ge ₇ Hf ₃ Ni ₁₀	20	-5.823	-6.163	0.000e+00	0.00709	0.635	2.068
snh_002_04853	Cs ₈ Dy ₆	14	-1.792	-1.996	-1.200e-05	0.0027	1.473	1.628
snh_002_04872	Cs ₃ Rb ₃ Tb ₆	12	-1.946	-2.235	-5.000e-06	0.00447	1.562	2.872
snh_002_04884	Ru ₁₀ Zr ₇	17	-8.843	-9.139	-1.000e-05	0.00824	0.886	1.023
snh_002_04895	Fe ₆ Ga ₂ LaSb ₂ Sr ₃	14	-5.005	-5.282	-8.000e-06	0.00566	0.803	0.674
snh_002_04949	Cs ₈ Nd ₆	14	-1.875	-2.122	-1.200e-05	0.0024	2.138	3.187
snh_002_04955	Ga ₂ Ni ₁₂ Si ₃ Sr	18	-5.159	-5.27	-2.100e-05	0.0096	0.241	1.034
snh_002_05029	Co ₆ Ge ₇ Sn	14	-5.037	-5.554	2.000e-06	0.00787	0.794	1.363
snh_003_00019	Co ₇ Sn ₈	15	-4.944	-5.238	-2.500e-05	0.00832	0.484	1.451
snh_003_00053	Co ₇ LiSn ₆	14	-4.86	-5.2	5.000e-06	0.00617	0.611	2.797
snh_003_00085	Al ₇ Ni ₈	15	-4.787	-5.166	-2.200e-05	0.00594	1.063	1.862
snh_003_00146	Co ₇ EuSn ₃	11	-5.193	-5.607	-5.000e-06	0.00927	0.259	2.885
snh_003_00181	NdNi ₁₃ Sn ₂	16	-5.136	-5.258	-2.000e-06	0.00552	0.34	0.348
snh_003_00294	Mn ₆ Sn ₇	13	-5.433	-5.898	-3.000e-06	0.0038	0.523	0.776
snh_003_00309	Cs ₅ Yb ₆	11	-0.836	-0.968	-2.000e-06	0.00134	1.524	1.083
snh_003_00333	AgCaLiNi ₈ Sn ₃	14	-4.095	-4.53	-1.900e-05	0.00735	1.018	1.355
snh_003_00372	Co ₆ Sn ₈	14	-4.638	-5.071	0.000e+00	0.00536	0.457	0.868
snh_003_00378	Co ₈ La ₂ Se ₄ Si	15	-5.587	-5.977	-2.000e-06	0.00573	1.069	1.683
snh_003_00415	Cs ₈ Gd ₆	14	-1.933	-2.035	-7.000e-06	0.00466	0.979	1.701
snh_003_00418	Eu ₂ Ge ₄ Ni ₈	14	-4.783	-5.08	-2.100e-05	0.00868	1.044	1.228
snh_003_00437	Ni ₇ Sn ₈	15	-4.472	-4.693	-1.500e-05	0.00758	0.725	1.098

Table S12. The profile of generated materials with Snub hexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
snh_003_00445	BaEuNi ₈ Sn ₂	12	-4.527	-4.746	-4.000e-06	0.00781	0.749	0.721
snh_003_00473	Al ₆ CsFe ₇	14	-5.206	-5.519	1.000e-06	0.00386	0.719	1.302
snh_003_00516	CoNi ₆ Sn ₇	14	-4.617	-4.769	-1.000e-06	0.0066	0.342	1.54
snh_003_00525	Cs ₂ Ru ₈ Sn ₅	15	-5.602	-6.002	0.000e+00	0.00767	0.494	0.925
snh_003_00529	Ni ₁₀ Sn ₅	15	-4.633	-5.063	-6.000e-06	0.00447	1.123	1.503
snh_003_00537	Cs ₆ RbYb ₇	14	-0.824	-0.979	-2.000e-06	0.00206	1.911	3.066
snh_003_00578	CoNdRu ₆ Sn ₇	15	-5.884	-6.241	-6.000e-06	0.00739	0.699	0.686
snh_003_00583	Co ₆ Sn ₆ Tl ₂	14	-4.613	-4.785	9.000e-06	0.00663	0.496	0.495
snh_003_00589	Co ₆ Sn ₈	14	-4.955	-5.074	0.000e+00	0.00629	0.412	0.539
snh_003_00661	Fe ₈ Te ₈	16	-5.11	-5.607	-4.800e-05	0.00991	1.123	1.399
snh_003_00758	AgAs ₄ Cs ₂ Ru ₇	14	-5.777	-6.121	-9.000e-06	0.006	0.976	1.867
snh_003_00771	K ₂ Mn ₆ Se ₄	12	-5.401	-5.975	0.000e+00	0.009	1.412	1.031
snh_003_00804	Ce ₃ GeIRu ₈ Sn	14	-6.88	-7.27	-1.000e-05	0.00785	1.124	1.332
snh_003_00838	Ge ₂ Mn ₈ SbSn ₃ Ti	15	-6.357	-6.721	1.000e-05	0.00851	1.126	1.116
snh_003_00932	Na ₃ Ni ₇ Sn	11	-3.864	-4.087	-3.000e-06	0.00568	1.048	0.929
snh_003_00959	GeMn ₆ Se ₃ Tl ₄	14	-4.983	-5.376	1.000e-06	0.00768	0.668	2.309
snh_003_00967	Cs ₈ Nd ₆	14	-1.84	-2.137	3.000e-06	0.00286	1.418	3.771
snh_003_00972	Ge ₂ Mn ₈ Sn ₆	16	-5.403	-6.206	-7.000e-06	0.00735	0.806	1.382
snh_003_01068	Co ₆ Se ₆	12	-5.076	-5.428	-5.000e-06	0.0097	0.708	1.736
snh_003_01161	Mn ₆ Sn ₅ Tl ₃	14	-4.83	-5.343	2.000e-06	0.00689	1.045	1.089
snh_003_01188	Al ₂ Mn ₆ Sn ₆	14	-5.395	-5.803	6.000e-06	0.00494	1.474	1.574
snh_003_01193	Co ₆ Sb ₂ SnTe ₅	14	-4.789	-5.051	2.000e-06	0.008	0.973	1.189
snh_003_01222	La ₅ Ru ₆ Si ₃	14	-6.952	-7.183	0.000e+00	0.00927	0.515	2.378
snh_003_01234	AllLa ₂ Mn ₇ P ₄ Sn	15	-6.677	-7.198	-2.000e-05	0.00739	0.822	0.899
snh_003_01254	Co ₆ Sn ₈	14	-4.912	-5.072	3.000e-06	0.00862	0.575	1.676
snh_003_01325	Al ₄ Ba ₂ Ge ₂ Ni ₆	14	-4.241	-4.599	-1.000e-06	0.00505	0.714	0.938
snh_003_01334	Al ₇ EuFe ₆	14	-5.216	-5.54	-2.100e-05	0.00777	0.654	0.596
snh_003_01401	Al ₃ CsLiNi ₆ Sr	12	-3.853	-4.085	0.000e+00	0.0065	1.3	2.246
snh_003_01452	Cs ₃ Ru ₆ Sn ₅	14	-4.886	-5.248	-3.000e-06	0.00585	0.877	1.481
snh_003_01470	Co ₉ DyGe ₂ In ₂ LaSn	16	-5.42	-5.72	-1.300e-05	0.00749	0.779	1.367
snh_003_01508	AuGeNa ₂ Ni ₆ Sn	11	-4.034	-4.287	-9.000e-06	0.00494	0.333	0.981
snh_003_01513	AsKMn ₆ Se ₆	14	-5.361	-5.956	2.000e-06	0.00794	0.874	2.145
snh_003_01567	Cs ₆ Yb ₆	12	-0.825	-0.936	2.000e-06	0.00232	1.223	2.763
snh_003_01685	Mn ₆ Sn ₆	12	-5.182	-6.079	0.000e+00	0.00836	1.393	2.771
snh_003_01704	Co ₈ Sn ₈	16	-4.89	-5.283	-2.000e-06	0.00648	0.592	1.435
snh_003_01711	P ₂ Ru ₆ Tl ₂	10	-6.12	-6.949	-4.000e-06	0.00664	1.417	1.643
snh_003_01740	CsIRu ₆ Te ₃	11	-5.068	-5.855	0.000e+00	0.00801	1.518	1.512
snh_003_01852	Ce ₆ Co ₆ Nd ₂	14	-6.167	-6.337	-7.000e-06	0.00744	0.987	0.917
snh_003_01860	Al ₈ Ni ₆	14	-4.494	-4.946	-4.400e-05	0.00682	0.806	2.306
snh_003_01909	Al ₃ Eu ₂ Ni ₆ Sn	12	-4.319	-4.63	-1.100e-05	0.00798	0.796	1.994
snh_003_01928	Ni ₈ Se ₈	16	-4.393	-4.708	-4.000e-06	0.00663	1.002	1.638
snh_003_01974	Cs ₆ Yb ₆	12	-0.814	-0.887	-	0.00955	1.927	5.314
					3.949e+01			
snh_003_01995	CaCog ₈ Ge ₈ Nd ₂	19	-5.42	-5.615	0.000e+00	0.00941	0.498	1.139
snh_003_02006	CdCs ₅ Yb ₆	12	-0.927	-1.0	-1.280e-04	0.00917	0.799	1.843
snh_003_02049	Ru ₆ Sn ₅ Sr ₃	14	-5.408	-5.776	0.000e+00	0.00422	1.111	1.43
snh_003_02056	CaNi ₇ Sn ₄	12	-4.388	-4.786	-3.000e-06	0.00809	0.997	1.537
snh_003_02112	Al ₃ Ge ₆ Ru ₁₁	20	-6.802	-7.105	0.000e+00	0.00705	0.472	1.001
snh_003_02172	AsCe ₂ Ga ₃ Ni ₆	12	-5.077	-5.268	8.000e-06	0.00676	1.504	1.09
snh_003_02214	Ba ₂ Mn ₆ Sn ₅	13	-5.326	-5.814	3.000e-06	0.00972	0.379	1.85
snh_003_02286	As ₂ CsRu ₆ Sb ₃	12	-5.913	-6.343	7.000e-06	0.00633	0.761	0.594
snh_003_02293	Mn ₆ RuSn ₈	15	-5.692	-5.993	-5.000e-06	0.00778	0.85	1.949

Table S12. The profile of generated materials with Snub hexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
snh_003_02386	Co ₇ Sn ₄ Sr	12	-5.057	-5.381	6.000e-06	0.00698	0.731	0.755
snh_003_02392	Li ₅ Mn ₆ Sn ₃	14	-4.821	-5.248	-2.000e-06	0.00635	1.449	1.625
snh_003_02398	CoLiMn ₆ PdSn ₇	16	-5.466	-5.778	0.000e+00	0.00609	0.905	1.737
snh_003_02626	Mn ₆ Sn ₄ Tl ₂	12	-5.344	-5.8	-5.000e-06	0.00455	0.951	0.747
snh_003_02675	Na ₂ Ni ₆ Sn ₃	11	-4.094	-4.279	0.000e+00	0.00485	1.443	1.086
snh_003_02682	Mn ₆ Rb ₂ Se ₄	12	-5.284	-5.94	4.000e-06	0.00707	1.628	2.214
snh_003_02690	Cs ₈ Dy ₆	14	-1.895	-1.995	1.000e-06	0.00364	1.256	1.932
snh_003_02721	Mn ₆ PtSn ₅	12	-5.53	-6.357	1.000e-06	0.00637	0.599	1.265
snh_003_02778	BaCo ₈ GeLi ₂	12	-4.81	-5.3	-2.800e-05	0.00501	1.003	2.803
snh_003_02787	Cs ₃ Ni ₇ Sn ₄	14	-3.843	-3.999	0.000e+00	0.00938	0.973	1.139
snh_003_02820	I ₆ Ru ₆	12	-4.461	-4.884	-2.000e-06	0.00694	0.842	1.509
snh_003_02823	Co ₆ GaGeSn ₂ Sr ₄	14	-4.245	-4.625	-1.000e-05	0.00937	0.621	0.831
snh_003_02842	Ni ₇ SiSn ₄	12	-4.628	-5.089	1.000e-06	0.00633	0.801	1.637
snh_003_02871	Ru ₆ Sn ₂ Tl ₂	10	-5.463	-6.358	6.000e-06	0.00308	1.202	1.038
snh_003_02974	Cs ₆ Rb ₃ Tb ₆	15	-1.741	-1.952	-3.000e-06	0.00496	1.437	2.344
snh_003_03017	Co ₆ Sn ₄ SrTl	12	-4.74	-5.034	-8.000e-06	0.00578	0.576	0.502
snh_003_03160	AlGaMn ₆ Sn ₄	12	-5.532	-6.172	-2.600e-05	0.00604	0.924	1.872
snh_003_03176	Mn ₆ Sn ₇	13	-5.574	-5.895	3.000e-06	0.00673	0.756	0.743
snh_003_03199	Cs ₃ Dy ₆	9	-2.473	-2.582	0.000e+00	0.00481	0.453	0.502
snh_003_03205	Al ₃ Co ₆ SnTb ₃	13	-5.228	-5.57	1.000e-06	0.00709	0.91	1.542
snh_003_03214	Al ₂ GeNi ₈ Sb ₂ Tb	14	-4.779	-5.135	-8.000e-06	0.00547	0.847	1.084
snh_003_03216	Cs ₈ SbTb ₆	15	-1.976	-2.211	-1.400e-05	0.00336	1.548	1.398
snh_003_03222	Rb ₂ Ru ₆ Se ₄	12	-5.395	-5.853	-2.500e-05	0.00826	0.821	0.779
snh_003_03242	Cs ₅ Tb ₆	11	-2.138	-2.307	1.600e-05	0.00679	0.715	0.743
snh_003_03278	Br ₆ Mn ₆	12	-4.716	-5.254	-2.000e-06	0.00865	1.137	1.261
snh_003_03284	Al ₂ Ge ₅ LaMgMn ₆	15	-5.703	-6.054	-1.100e-05	0.00608	0.797	0.758
snh_003_03363	Mn ₆ Sn ₃	9	-6.162	-6.859	0.000e+00	0.00803	0.967	0.487
snh_003_03367	Ba ₂ Ga ₆ Ni ₈	16	-4.15	-4.331	0.000e+00	0.00594	0.988	1.214
snh_003_03392	Ni ₁₀ Sn ₇	17	-4.694	-4.893	-4.000e-06	0.00733	0.584	1.223
snh_003_03464	GeRu ₆ Sn ₂ Tl ₂	11	-5.705	-6.291	0.000e+00	0.00708	1.197	1.372
snh_003_03512	Ni ₆ Sn ₆	12	-3.943	-4.79	-2.000e-06	0.00641	0.439	1.077
snh_003_03518	Ru ₁₅ Sn ₅	20	-7.271	-7.718	0.000e+00	0.00487	0.709	0.642
snh_003_03536	Ce ₈ Fe ₉ Ga	18	-6.754	-7.024	0.000e+00	0.00687	0.541	2.039
snh_003_03569	AlRu ₁₀ Sm ₂ Tb	14	-7.426	-7.789	0.000e+00	0.00558	0.629	1.4
snh_003_03582	BaGe ₂ Ni ₉	12	-4.838	-5.075	-3.000e-06	0.00536	0.852	1.079
snh_003_03645	K ₄ Ru ₆ Sn ₄	14	-4.85	-5.168	0.000e+00	0.00603	1.41	1.255
snh_003_03647	GaGe ₂ Mn ₆ Sn ₅	14	-5.574	-5.902	0.000e+00	0.00336	0.159	1.073
snh_003_03687	K ₂ Mn ₆ Sn ₂	10	-5.122	-5.971	0.000e+00	0.00416	1.559	3.075
snh_003_03705	Ru ₇ Sn ₆ Sr ₂	15	-5.831	-6.065	-1.000e-06	0.00638	0.403	1.453
snh_003_03711	BrCl ₈ Ru ₆	15	-4.366	-4.798	-8.000e-06	0.00923	0.968	1.639
snh_003_03777	GeMn ₆ PSn ₆	14	-4.697	-5.996	0.000e+00	0.00622	0.72	0.772
snh_003_03821	Al ₇ EuRu ₆	14	-5.75	-6.236	-2.000e-06	0.00567	1.302	2.019
snh_003_03823	ErFe ₈ GeNbSi ₇	18	-6.572	-6.995	1.000e-05	0.00756	0.46	1.251
snh_003_03844	Ba ₃ Ni ₆ Sn ₄	13	-4.24	-4.404	-3.000e-06	0.00699	0.961	1.595
snh_003_03906	Fe ₆ Se ₆ Tl ₂	14	-5.106	-5.438	-2.100e-05	0.00717	0.665	1.213
snh_003_03914	BaCuFe ₆ GaSn ₅	14	-5.036	-5.361	-1.000e-05	0.0045	0.954	1.439
snh_003_03971	Ge ₃ Ni ₇ SrTm	12	-4.791	-5.163	5.000e-06	0.00458	1.334	1.103
snh_003_04018	Mn ₆ Sn ₈	14	-5.381	-5.768	-4.000e-06	0.00591	0.653	1.856
snh_003_04083	Ni ₁₀ Sn ₇ Zn	18	-4.401	-4.644	-1.000e-06	0.00593	0.691	1.159
snh_003_04086	Ca ₃ GaN ₈ Sn ₂	14	-4.267	-4.479	-2.000e-06	0.00618	0.919	1.432
snh_003_04133	Cs ₄ Yb ₆	10	-0.831	-0.966	4.000e-07	0.00153	1.011	1.049
snh_003_04183	Cs ₅ Yb ₆	11	-0.801	-0.968	-7.900e-05	0.00997	0.961	2.041

Table S12. The profile of generated materials with Snub hexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
snh.003_04200	Co ₅ Ni ₈ Si ₃ Zr	17	-5.956	-6.285	0.000e+00	0.00975	1.072	0.885
snh.003_04223	Mn ₆ Se ₆	12	-5.852	-6.452	-3.000e-06	0.00799	0.706	0.835
snh.003_04248	Ni ₆ Sn ₆	12	-4.513	-4.709	1.000e-06	0.00641	0.741	0.784
snh_003_04251	Mn ₈ Si ₁₁ Ti	20	-6.814	-7.095	1.000e-05	0.00762	0.755	1.068
snh_003_04282	Cs ₈ Nd ₆	14	-1.977	-2.134	0.000e+00	0.00486	1.429	1.882
snh_003_04313	Ce ₂ GeNdNi ₁₁	15	-5.433	-5.679	0.000e+00	0.00692	0.496	1.517
snh_003_04412	Cs ₈ Yb ₆	14	-0.849	-0.953	-1.000e-05	0.00217	1.186	1.476
snh_003_04440	Co ₆ LaSr ₇	14	-3.629	-3.949	-1.400e-05	0.00526	0.857	1.086
snh_003_04458	Ge ₂ In ₂ Mn ₈ Tm ₃	15	-6.045	-6.525	-3.000e-06	0.00692	1.135	2.027
snh.003_04495	Ru ₆ Sn ₆ Sr ₂	14	-5.39	-5.812	1.000e-06	0.00661	0.915	0.765
snh_003_04588	Co ₆ Na ₃	9	-4.066	-4.553	-5.000e-06	0.0069	1.758	1.451
snh_003_04617	Mn ₆ Sn ₈	14	-5.513	-5.775	-3.000e-06	0.00826	0.762	1.668
snh_003_04675	Cs ₆ Nd ₆	12	-2.222	-2.346	-1.000e-06	0.0028	1.453	1.91
snh.003_04729	Fe ₆ Ga ₆ Sm ₂	14	-5.191	-5.534	-5.000e-06	0.0044	0.528	0.679
snh_003_04793	GeNi ₆ Te ₆ Zn	14	-3.928	-4.195	-5.000e-06	0.00838	0.987	1.502
snh_003_04811	Ru ₁₀ Sn ₃ Y ₂	15	-7.296	-7.743	0.000e+00	0.00625	0.966	1.045
snh_003_04960	CrFe ₇ NbSi ₁₁	20	-6.717	-7.016	0.000e+00	0.00713	0.515	1.211
snh_004_00020	BaGa ₂ Ni ₆ Sn ₄	13	-4.196	-4.429	0.000e+00	0.00618	0.489	1.699
snh_004_00031	Cs ₅ Yb ₆	11	-0.782	-0.968	0.000e+00	0.00182	0.864	1.068
snh_004_00080	NdRu ₈ Sn ₄	13	-6.712	-7.125	-5.000e-06	0.00759	0.442	1.597
snh_004_00110	Ni ₆ Sn ₈	14	-4.509	-4.631	-6.000e-06	0.00615	0.62	0.697
snh_004_00119	Cs ₈ Tb ₆	14	-1.681	-2.018	0.000e+00	0.00335	1.897	3.248
snh_004_00133	Ce ₅ Co ₉ Ge ₂	16	-6.361	-6.616	0.000e+00	0.00841	0.726	1.929
snh_004_00151	Ni ₇ Sn ₆	13	-3.971	-4.868	-1.700e-05	0.00971	0.419	1.16
snh_004_00172	Ca ₃ Co ₆	9	-4.752	-5.127	-1.500e-05	0.00802	0.497	1.311
snh_004_00207	As ₂ GeMn ₇ Rb ₂	12	-5.54	-6.295	-7.000e-06	0.00719	2.149	1.855
snh_004_00240	Ni ₆ Sn ₄	10	-4.402	-4.912	1.000e-06	0.00679	0.706	2.716
snh_004_00243	BaCo ₇ Sn ₆	14	-4.711	-5.185	-3.000e-06	0.00662	0.855	1.555
snh_004_00308	Cs ₇ Dy ₆	13	-1.988	-2.077	-8.000e-06	0.00229	0.779	2.263
snh.004_00361	Co ₈ Gd ₂ Sn ₃	13	-5.585	-5.935	-1.000e-06	0.0089	0.706	0.696
snh.004_00373	Fe ₆ Se ₆	12	-5.615	-5.948	-1.300e-05	0.00779	0.387	0.365
snh.004_00405	Ru ₁₆ Zr ₄	20	-8.817	-9.061	1.000e-05	0.00558	0.34	0.739
snh_004_00472	Ru ₆ Sn ₈	14	-5.699	-5.991	-1.000e-06	0.00452	0.745	1.259
snh.004_00629	Ru ₆ Sn ₄ Tl ₂	12	-5.594	-5.963	0.000e+00	0.00461	0.578	0.524
snh_004_00694	Cs ₅ Tb ₆	11	-2.236	-2.306	-3.000e-06	0.00324	0.418	2.136
snh.004_00762	Ce ₂ Ge ₃ Mn ₇ Pt	13	-6.926	-7.37	-4.000e-06	0.00677	0.613	0.632
snh_004_00776	GeNi ₆ Tl ₆	13	-3.54	-3.726	-1.000e-06	0.00877	0.982	1.755
snh_004_00811	Cs ₅ Yb ₆	11	-0.844	-0.968	0.000e+00	0.00326	1.123	1.687
snh.004_00827	GeKNi ₆ Sn ₂ Tl	11	-4.083	-4.311	-6.000e-06	0.00858	0.665	0.747
snh.004_00833	AuRu ₆ Se ₅ Tl	13	-5.333	-5.911	0.000e+00	0.00554	0.796	0.997
snh_004_00849	Mn ₆ SiTe ₇	14	-4.967	-5.629	-5.000e-06	0.00703	1.125	1.226
snh.004_00930	AlLa ₆ Ni ₆	13	-5.091	-5.303	2.000e-06	0.00787	0.658	0.802
snh_004_00962	Fe ₇ Nd ₂ SiZn ₄	14	-5.044	-5.401	-2.300e-05	0.00536	0.967	1.75
snh.004_00976	AuEuMn ₆ Sn ₄	12	-5.653	-6.066	-1.000e-06	0.00545	0.761	0.802
snh.004_01023	Co ₆ GaSn ₇	14	-4.479	-5.073	2.000e-06	0.00656	1.014	0.889
snh_004_01036	GaNdNi ₈ Sn ₄	14	-4.788	-4.97	-2.000e-06	0.00686	0.879	1.672
snh.004_01162	Al ₂ Mn ₉ Si ₈ Ti	20	-6.782	-7.154	0.000e+00	0.00553	0.416	0.904
snh.004_01197	Ge ₃ La ₂ Ni ₇	12	-5.231	-5.489	-1.000e-06	0.00914	0.547	0.603
snh_004_01278	Ce ₄ Ni ₆ Sr	11	-5.045	-5.421	-4.000e-06	0.00605	0.9	1.492
snh_004_01280	Ni ₆ Sn ₅ Sr ₂	13	-4.379	-4.437	-3.000e-06	0.00746	0.171	1.86
snh_004_01308	AgFe ₆ Se ₇	14	-5.2	-5.594	-6.000e-06	0.00674	0.991	1.644
snh.004_01319	Ni ₆ Sn ₇ Y	14	-4.763	-4.953	-3.000e-06	0.00558	0.58	0.591

Table S12. The profile of generated materials with Snub hexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
snh_004_01392	La ₄ Ni ₁₁	15	-5.245	-5.485	1.000e-06	0.00861	0.732	1.2
snh_004_01409	Ni ₆ Sn ₈	14	-4.402	-4.633	-1.500e-05	0.00994	0.349	1.337
snh_004_01488	Ru ₁₃ Sn ₅ Zr	19	-7.031	-7.62	-3.000e-05	0.0078	0.486	1.996
snh_004_01489	Fe ₇ Ga ₂ La ₂	11	-6.15	-6.558	0.000e+00	0.00577	0.691	1.82
snh_004_01500	AgCaMn ₆ P ₂ Sn ₂	12	-5.718	-6.349	-4.000e-06	0.00446	0.952	1.851
snh_004_01509	Ni ₇ Sn ₅	12	-4.528	-4.877	-5.000e-06	0.0068	0.304	1.103
snh_004_01524	Co ₇ HfLaSi ₈	17	-6.342	-6.664	0.000e+00	0.00919	0.879	2.286
snh_004_01585	Ni ₆ Sn ₅ Sr ₃	14	-3.733	-4.351	-2.000e-06	0.00613	0.656	1.231
snh_004_01665	Mn ₈ SbSn ₅	14	-6.008	-6.41	-4.000e-06	0.00469	0.738	0.777
snh_004_01704	Al ₅ GeNi ₆ SrU	14	-4.78	-5.212	-5.000e-06	0.0068	1.065	1.424
snh_004_01725	La ₃ Mn ₆ Sb ₄ Sr	14	-6.068	-6.375	-7.000e-06	0.00707	1.106	1.493
snh_004_01737	I ₆ Ni ₆	12	-3.231	-3.444	-8.000e-06	0.00752	0.662	1.42
snh_004_01747	Br ₄ ClIRu ₆	12	-4.422	-5.179	0.000e+00	0.00508	1.227	1.641
snh_004_01772	Cs ₅ Tb ₆	11	-1.933	-2.307	4.000e-06	0.00333	1.383	2.117
snh_004_01838	Al ₂ Co ₁₀ Y ₃	15	-6.282	-6.539	-6.000e-06	0.00509	0.688	1.007
snh_004_01856	BaMn ₆ Sn ₆ Zr	14	-5.789	-6.163	2.000e-06	0.00574	0.736	0.746
snh_004_01998	Co ₆ Sn ₈ Sr ₂	16	-4.418	-4.795	1.500e-05	0.00919	0.69	1.024
snh_004_02007	Mn ₆ Sn ₆ Sr ₂	14	-5.292	-5.698	0.000e+00	0.00414	0.473	1.699
snh_004_02009	Fe ₆ Se ₆	12	-5.452	-5.981	-4.000e-06	0.00746	0.459	1.305
snh_004_02024	Co ₉ Pr ₃ Sn ₂	14	-5.726	-6.003	3.000e-06	0.00964	0.467	1.014
snh_004_02102	Ni ₆ Sn ₆	12	-4.375	-4.794	-5.000e-06	0.00643	0.462	1.244
snh_004_02127	Ni ₆ Sn ₄ Sr ₄	14	-4.034	-4.226	-1.400e-05	0.00912	0.577	0.697
snh_004_02146	Co ₁₆ Nd ₃	19	-6.138	-6.442	1.000e-05	0.00999	1.048	0.931
snh_004_02181	Ni ₁₂ Pr ₂	14	-5.144	-5.429	1.000e-06	0.00719	0.846	1.088
snh_004_02209	K ₄ Mn ₆ Sn ₃	13	-4.454	-5.021	2.000e-06	0.00865	1.739	2.465
snh_004_02291	Cs ₅ Yb ₆	11	-0.826	-0.967	-7.000e-06	0.00448	1.167	3.977
snh_004_02295	AlCoGe ₅ Mn ₇ RuScSi ₄	20	-6.422	-6.717	0.000e+00	0.00887	0.758	1.264
snh_004_02341	AuNi ₈ Sn ₂	11	-4.604	-5.001	-7.000e-06	0.0079	1.27	1.4
snh_004_02351	Mn ₆ RuSn ₅	12	-6.022	-6.547	-6.000e-05	0.0095	0.648	1.244
snh_004_02476	Cs ₂ Mn ₆ Te ₄	12	-5.256	-5.566	-1.000e-06	0.00947	0.474	0.434
snh_004_02592	NdRu ₈ Sn ₅	14	-6.221	-6.837	-1.000e-06	0.00937	0.59	0.624
snh_004_02615	Ca ₆ Ru ₈	14	-5.449	-5.912	-2.000e-06	0.00751	1.067	1.334
snh_004_02622	Cs ₆ Nd ₆	12	-2.048	-2.35	-4.000e-06	0.00345	1.642	2.852
snh_004_02698	Al ₅ Fe ₈ Si ₂	15	-5.905	-6.507	-5.900e-05	0.00951	0.779	1.177
snh_004_02720	Ru ₁₁ Sn ₈	19	-6.006	-6.752	0.000e+00	0.00703	0.425	2.455
snh_004_02736	BaMn ₆ Sn ₈	15	-5.266	-5.632	0.000e+00	0.0061	0.77	1.514
snh_004_02774	Fe ₆ Se ₆	12	-5.53	-5.981	-3.000e-06	0.00762	0.61	0.663
snh_004_02917	AlNi ₁₆ Sc	18	-5.275	-5.468	2.000e-06	0.00625	0.438	0.673
snh_004_02955	Ba ₂ Mn ₇ SbSn ₃	13	-5.372	-6.149	3.000e-06	0.00578	1.194	2.136
snh_004_02994	Ba ₂ Ni ₆ Sn ₄	12	-4.325	-4.551	-1.900e-05	0.00823	0.759	0.83
snh_004_03117	Co ₆ Ga ₃ Y ₅	14	-5.913	-6.106	-1.300e-05	0.00614	0.482	0.546
snh_004_03121	Ce ₂ EuRu ₇ Sn ₂	12	-6.763	-7.173	-1.000e-06	0.00635	0.798	1.326
snh_004_03222	Ru ₁₆ Sn ₄	20	-7.094	-7.947	0.000e+00	0.00443	0.31	1.496
snh_004_03248	Ni ₆ Sn ₇	13	-4.392	-4.667	0.000e+00	0.00783	0.695	0.767
snh_004_03276	AlGeMn ₆ Sn ₈	16	-5.026	-5.569	2.000e-06	0.00516	1.222	1.866
snh_004_03346	NdRu ₇ SbSn ₁₀	19	-5.393	-5.847	0.000e+00	0.00472	0.844	1.663
snh_004_03386	AgMn ₆ Sn ₇	14	-5.426	-5.678	3.000e-06	0.00562	0.42	1.499
snh_004_03405	Co ₆ Ga ₇ Nd ₂	15	-4.774	-5.053	-3.000e-06	0.00743	0.516	1.925
snh_004_03447	Ru ₇ Sn ₈	15	-5.925	-6.268	1.000e-06	0.00726	0.719	0.981
snh_004_03478	Cs ₅ Tb ₆	11	-2.201	-2.307	-1.600e-05	0.00381	0.634	0.541
snh_004_03589	Mn ₇ Sn ₆	13	-5.914	-6.278	-1.000e-05	0.00791	0.387	0.594
snh_004_03596	Na ₄ Ni ₆ Sn ₃	13	-3.739	-3.838	-1.000e-06	0.00893	0.554	1.366

Table S12. The profile of generated materials with Snub hexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
snh_004_03707	Mn ₆ Sn ₆ Sr	13	-5.363	-5.866	-1.000e-06	0.0041	0.987	2.278
snh_004_03709	Fe ₇ GaN ₁₀	18	-3.269	-3.617	0.000e+00	0.00557	1.417	1.614
snh_004_03735	Ni ₆ Sn ₅ SrY ₂	14	-4.914	-5.124	7.000e-06	0.00524	0.285	0.497
snh_004_03818	Mn ₇ PdSn ₆	14	-5.546	-6.194	0.000e+00	0.00692	0.722	1.674
snh_004_03821	CeCo ₁₁ Ge ₅	17	-5.976	-6.259	-1.000e-05	0.00903	0.578	1.081
snh_004_03853	Co ₇ GeSn ₇	15	-4.884	-5.264	-7.000e-06	0.00904	0.801	1.217
snh_004_03919	FeMn ₁₁ Si ₇ Tc	20	-7.502	-7.953	-1.000e-05	0.00765	0.563	0.878
snh_004_04124	EuRu ₆ Sn ₃ Tl ₄	14	-5.109	-5.37	-7.000e-06	0.00953	0.708	1.699
snh_004_04161	Co ₆ Cs ₃	9	-3.874	-4.095	-1.300e-05	0.00935	0.987	0.88
snh_004_04177	Ni ₇ PSn ₅	13	-4.682	-4.97	-1.000e-06	0.00728	1.113	1.407
snh_004_04197	AlCo ₆ GeZr ₅	13	-6.943	-7.392	-1.000e-05	0.00632	1.01	3.088
snh_004_04253	Co ₇ Na ₄	11	-4.187	-4.431	0.000e+00	0.00721	0.691	0.576
snh_004_04294	Al ₃ Fe ₇ NdSi ₂ Sr	14	-5.842	-6.213	-2.100e-05	0.00793	0.957	0.992
snh_004_04311	Mn ₆ Sn ₆	12	-5.672	-5.974	0.000e+00	0.0088	1.035	2.006
snh_004_04312	Al ₄ Ru ₆ SnSr ₃	14	-5.158	-5.642	-1.000e-06	0.00452	0.945	0.856
snh_004_04399	Ge ₅ Ru ₁₀ Zr ₅	20	-7.546	-8.1	-1.000e-05	0.00531	0.612	1.064
snh_004_04404	Ru ₆ Se ₆	12	-5.929	-6.383	-6.000e-06	0.00469	0.615	0.61
snh_004_04413	Co ₆ Ge ₂ Sr ₂	10	-4.932	-5.427	-3.500e-05	0.00517	1.269	1.314
snh_004_04422	Co ₈ Eu ₂ Ge ₃ Sn	14	-5.439	-5.673	-6.000e-06	0.00643	0.496	1.359
snh_004_04462	CoMn ₆ Sn ₅	12	-5.613	-6.37	3.000e-06	0.00641	0.616	1.885
snh_004_04584	Co ₆ Zr ₈	14	-7.834	-8.071	-1.000e-05	0.00809	0.561	1.048
snh_004_04643	Ni ₆ Se ₆	12	-4.267	-4.707	-9.000e-06	0.0074	0.51	0.826
snh_004_04733	Ru ₁₂ Sn ₇	19	-6.507	-7.036	-1.000e-05	0.00846	0.586	0.805
snh_004_04765	Br ₆ Ru ₆	12	-4.445	-5.138	3.000e-06	0.00733	1.114	1.143
snh_004_04801	Co ₆ I ₂ Se ₅	13	-4.572	-4.868	1.800e-05	0.00991	0.526	0.517
snh_004_04923	Fe ₆ Sn ₆	12	-5.432	-5.73	0.000e+00	0.00684	0.838	0.694
snh_004_04975	Al ₂ Fe ₆ La ₂ Si ₃	13	-6.102	-6.474	-2.000e-06	0.00587	0.631	0.591
snh_004_04994	Ni ₉ Sb ₂ Sn ₅	16	-4.454	-4.85	-1.000e-06	0.00902	0.626	0.974
snh_004_05001	Al ₅ Ge ₂ Hf ₂ Ni ₇ Si	17	-5.431	-5.73	9.000e-06	0.00771	0.462	1.346
snh_004_05035	Ru ₆ Sn ₇ U	14	-6.335	-6.625	-4.900e-05	0.00693	0.612	1.381
snh_004_05042	Cs ₄ Yb ₆	10	-0.799	-0.982	4.500e-06	0.00318	1.749	1.789
snh_004_05067	Ru ₆ S ₂ Te	12	-5.911	-6.415	-2.400e-05	0.00653	0.415	0.639
snh_004_05095	Cs ₃ Tb ₆	9	-2.477	-2.86	0.000e+00	0.00887	3.745	2.463
snh_004_05143	Mn ₆ Rb ₃ Sn ₆	15	-4.762	-5.091	-2.000e-06	0.00626	0.534	1.799
snh_004_05149	BaGa ₇ Mn ₆	14	-5.012	-5.407	-2.200e-05	0.00861	0.456	1.289
snh_005_00021	Ni ₇ Sn ₃ Tl ₂	12	-4.25	-4.478	1.000e-06	0.00724	0.526	1.189
snh_005_00054	Ba ₄ Ru ₆ Sn ₄	14	-5.412	-5.682	-4.000e-06	0.00344	0.73	1.233
snh_005_00069	Co ₈ Ge ₂ HoPd ₄ Sn ₂	17	-5.477	-5.821	-1.000e-06	0.00542	0.69	1.12
snh_005_00119	Ga ₇ Ni ₇ SbY	16	-4.414	-4.628	-7.000e-06	0.00563	1.056	1.133
snh_005_00124	Mn ₁₂ P ₆ SiZr	20	-7.631	-8.092	0.000e+00	0.00898	0.658	1.367
snh_005_00180	Al ₈ Co ₆	14	-4.906	-5.282	-8.000e-06	0.00842	0.426	0.766
snh_005_00239	Cs ₆ Yb ₆	12	-0.885	-0.96	-8.000e-06	0.0039	2.189	2.553
snh_005_00311	Ni ₆ Sn ₉ Sr ₃	18	-3.944	-4.312	-1.000e-06	0.00976	0.448	1.514
snh_005_00324	BiCaGe ₂ Ni ₈	12	-4.793	-4.982	-9.800e-05	0.00896	0.413	0.921
snh_005_00326	Ga ₃ Ge ₂ Mn ₈ MoNiSn ₃	18	-5.977	-6.377	0.000e+00	0.00592	0.554	1.072

Table S13. The profile of generated materials with Truncated hexagonal lattice structures after DFT relaxation

Index	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
trh_000_00001	Mn ₆ SnTl ₈	15	-3.476	-4.535	-2.700e-05	0.00695	2.286	1.332
trh_000_00842	GaLa ₉ Ni ₆ Sn ₂	18	-4.87	-5.203	-1.600e-05	0.00692	0.892	1.23
trh_000_02190	Co ₆ Cs ₂ I ₈	16	-3.183	-3.538	-1.000e-05	0.00659	1.317	0.755
trh_000_02459	CdCo ₇ La ₆ SbSn ₅	20	-4.939	-5.354	1.000e-05	0.00736	1.422	1.748
trh_000_02609	BrCs ₂ I ₆ Mn ₇ Se	17	-3.939	-4.667	-7.000e-06	0.007	2.077	1.639
trh_000_02659	Ni ₆ Sn ₁₄	20	-3.914	-4.399	5.000e-06	0.00845	0.982	2.149
trh_001_00300	Cs ₁₁ Dy ₆	17	-1.307	-1.658	-3.700e-05	0.00726	2.953	2.894
trh_001_01144	Co ₆ In ₅ LuRb ₂ Sn ₆	20	-3.755	-4.191	2.000e-06	0.00655	1.387	2.003
trh_001_01344	ClCo ₆ I ₈ Tl	16	-3.148	-3.513	-2.100e-05	0.00654	1.159	1.603
trh_001_03111	Cs ₉ Gd ₆	15	-1.275	-1.953	-9.800e-05	0.00675	4.241	6.911
trh_002_00185	Cs ₁₀ Ru ₆	16	-2.463	-3.283	5.000e-06	0.00901	2.102	3.072
trh_002_00533	Co ₆ La ₄ Rb ₃ Sb ₇	20	-4.584	-4.912	-1.000e-05	0.00975	1.103	1.518
trh_002_00573	Mn ₇ Rb ₅ Sn ₅	17	-4.152	-4.687	-3.000e-06	0.00807	2.237	2.989
trh_002_00957	Cs ₁₁ Nd ₆ Sn	18	-1.537	-2.011	-2.600e-05	0.00486	2.713	2.454
trh_002_01132	Br ₁₁ CsRu ₆ Sn	19	-3.544	-4.286	-1.000e-06	0.00713	1.574	2.214
trh_002_01870	Br ₈ Co ₆ Cs ₂	16	-3.11	-3.757	-5.000e-06	0.00677	2.027	1.195
trh_002_02606	KNi ₇ Sn ₁₂	20	-3.897	-4.327	-4.000e-06	0.00934	1.191	1.581
trh_002_02688	Co ₆ Cs ₂ I ₈	16	-3.022	-3.557	-4.500e-05	0.00898	1.586	1.98
trh_002_02908	Cs ₁₄ Ru ₆	20	-2.136	-2.685	-1.000e-06	0.00477	2.237	1.864
trh_002_03095	Cs ₉ Nd ₆	15	-1.49	-2.047	-1.530e-04	0.00869	3.73	4.173
trh_003_00223	Br ₁₁ CsFeNi ₆	19	-3.19	-3.446	0.000e+00	0.00517	0.798	1.688
trh_003_00359	Cs ₁₁ Tb ₆	17	-1.264	-1.705	3.000e-06	0.00304	2.912	4.438
trh_003_00954	Co ₆ Te ₉	15	-4.066	-4.702	-7.200e-05	0.00892	1.444	1.246
trh_003_00975	Cs ₁₀ Nd ₆	16	-1.398	-1.886	-1.000e-06	0.00358	3.903	4.131
trh_003_01226	I ₈ Mn ₆ Sn	15	-3.821	-4.403	-3.700e-05	0.00706	1.711	2.39
trh_003_01255	Co ₆ NaTe ₇ Tl	15	-3.801	-4.446	-2.000e-06	0.00823	1.811	1.059
trh_003_01355	Co ₆ I ₈ Sn	15	-3.144	-3.612	-4.000e-06	0.00641	1.629	1.607
trh_003_02037	Cd ₂ Co ₆ Sn ₁₀ Tl	19	-3.753	-4.288	-1.000e-06	0.00833	1.817	2.206
trh_003_02061	Cs ₉ Dy ₆	15	-1.286	-1.867	-1.600e-05	0.00464	3.679	2.991
trh_003_02464	Cs ₁₁ Dy ₆	17	-1.241	-1.674	-2.600e-05	0.0086	1.56	3.517
trh_004_00380	AgCo ₆ I ₈ Na	16	-3.047	-3.491	-5.000e-06	0.00579	1.085	0.793
trh_004_01142	CdCo ₆ I ₉ La	17	-3.213	-3.66	-4.800e-05	0.00801	1.252	2.233
trh_004_01646	Co ₇ GeTe ₁₂	20	-3.971	-4.542	-5.000e-05	0.00809	1.465	1.045
trh_004_02633	Fe ₇ I ₉ La	17	-3.805	-4.289	-1.500e-05	0.00654	1.399	1.218
trh_004_02993	CsMn ₆ Sn ₈	15	-4.44	-5.482	0.000e+00	0.00574	2.59	5.296
trh_005_00195	Cs ₉ Mn ₆	15	-2.766	-3.203	-1.400e-05	0.00991	2.444	2.204
trh_005_00267	Br ₈ LaRu ₆	15	-4.211	-5.114	-7.000e-06	0.0059	1.966	2.326
trh_005_00625	Cs ₁₀ Tb ₆	16	-1.355	-1.689	-2.540e-04	0.00917	1.798	2.148
trh_005_00634	Mn ₇ Sn ₅ Tl ₅	17	-4.27	-5.053	1.500e-05	0.0088	2.159	1.484
trh_005_01790	I ₉ Mn ₆ STe	17	-3.616	-4.272	0.000e+00	0.00889	1.938	2.036
trh_005_02429	Cs ₈ Dy ₆	14	-1.381	-1.864	3.000e-06	0.00317	3.471	4.964
trh_006_00185	CsNi ₆ Sn ₁₂	19	-3.809	-4.252	-6.800e-05	0.00643	1.506	1.831
trh_006_00221	Br ₈ Co ₆ Cs ₂	16	-3.421	-3.75	1.300e-05	0.00957	1.138	1.203
trh_006_01078	GdNi ₆ SbSn ₁₀	18	-4.091	-4.6	-5.000e-06	0.0063	1.106	1.771
trh_006_01740	Br ₁₁ CoRu ₆	18	-3.529	-4.372	-2.100e-05	0.00848	1.589	1.169
trh_006_01777	Co ₆ Sb ₃ Sn ₁₀	19	-4.335	-4.832	-8.000e-06	0.0073	1.533	1.944
trh_006_01808	Co ₆ I ₈ La	15	-3.631	-3.982	-5.000e-06	0.00875	1.371	0.917
trh_006_01896	Cs ₉ Ru ₆ Sn	16	-2.559	-3.575	-7.000e-06	0.00516	2.634	2.519
trh_006_01950	CsI ₁₁ Mn ₆ Sn	19	-3.389	-4.014	1.300e-05	0.0064	1.189	1.012
trh_006_02087	Cs ₁₁ Nd ₆	17	-1.37	-1.839	-2.900e-05	0.00406	4.807	3.144
trh_006_02728	Ni ₆ Sn ₁₀ Tl	17	-3.863	-4.339	-1.900e-05	0.00587	1.082	1.826
trh_006_03020	AlBr ₁₁ Co ₆ CsGe	20	-3.429	-3.79	-2.700e-05	0.00814	0.772	1.397

Table S13. The profile of generated materials with Truncated hexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
trh_006_03251	I ₉ LaMn ₆	16	-3.854	-4.599	-1.100e-05	0.00957	1.67	1.191
trh_007_00319	Br ₁₁ Co ₆ LaTl	19	-3.581	-3.903	1.900e-05	0.0069	0.453	1.616
trh_007_01702	Fe ₆ I ₁₁ TeTl	19	-3.094	-3.565	2.000e-06	0.00785	1.789	1.63
trh_007_01875	Cs ₄ Fe ₆ Te ₈	18	-3.932	-4.423	5.000e-06	0.00653	0.861	3.588
trh_007_02587	Cs ₁₀ Dy ₆	16	-1.329	-1.715	-2.000e-06	0.00643	2.354	3.166
trh_007_02603	I ₈ Mn ₇ Se	16	-3.865	-4.72	-6.500e-05	0.00802	0.827	1.396
trh_008_00241	BaCo ₆ I ₁₀ Sn	18	-3.117	-3.566	-4.200e-05	0.00953	1.712	2.357
trh_008_01279	AgBr ₁₀ Fe ₆	17	-3.414	-3.971	-2.000e-06	0.0054	2.009	1.297
trh_008_01353	Cs ₁₀ Tb ₆	16	-1.351	-1.794	-1.100e-05	0.00367	2.379	5.352
trh_008_02246	La ₃ Ni ₆ Sn ₁₁	20	-4.362	-4.808	4.000e-06	0.0064	0.448	0.96
trh_008_02821	Br ₈ Co ₆ K ₂	16	-3.428	-3.776	-2.900e-05	0.00846	0.997	0.749
trh_008_03065	I ₈ NaNi ₇	16	-3.018	-3.29	1.000e-06	0.008	0.799	2.775
trh_008_03335	Bi ₆ Ce ₂ La ₂ Ru ₆ Sn ₄	20	-5.405	-5.943	-1.000e-05	0.00908	1.963	1.87
trh_009_01366	La ₇ LiNi ₈ Sn ₄	20	-4.848	-5.151	0.000e+00	0.00477	1.151	0.86
trh_009_01634	La ₆ Ni ₆ Sn ₈	20	-4.843	-5.11	0.000e+00	0.00822	1.093	1.117
trh_009_01819	Br ₂ Co ₆ La ₂ Se ₇ Te	18	-4.445	-5.109	-2.200e-05	0.00706	1.26	0.956
trh_009_01853	I ₁₀ Ni ₇ Zr	18	-3.268	-3.582	-2.700e-05	0.00672	1.45	1.662
trh_009_02805	Cs ₁₂ Ru ₆	18	-2.035	-2.942	-1.500e-05	0.00611	3.129	2.618
trh_010_01748	Cs ₉ SnTb ₆	16	-1.655	-1.987	3.000e-06	0.00637	1.509	2.909
trh_010_01875	Co ₆ CsHgI ₉ K	18	-2.989	-3.249	5.000e-06	0.00683	0.903	1.361
trh_010_01987	Ni ₇ Pr ₅ Sn ₇	19	-4.569	-5.087	-9.000e-06	0.00672	2.33	3.029
trh_010_02558	Co ₆ I ₉ RbSn	17	-3.07	-3.53	-3.000e-06	0.00672	1.18	1.52
trh_011_00632	Cs ₁₀ Tb ₆	16	-1.302	-1.677	-1.000e-05	0.00443	2.206	3.827
trh_011_01062	AgFe ₆ I ₁₀	17	-3.158	-3.749	-1.000e-06	0.00424	0.757	1.929
trh_011_01371	Br ₉ ClMn ₆ Te	17	-3.95	-4.463	-1.200e-05	0.00906	1.02	1.004
trh_011_01620	K ₄ Mn ₇ Sn ₉	20	-4.021	-4.834	-5.000e-06	0.0057	2.286	2.933
trh_011_01959	Al ₅ KLa ₈ Ni ₆	20	-4.524	-4.809	-1.000e-06	0.00816	1.595	2.54
trh_011_02020	I ₁₁ Mn ₇ Te	19	-3.595	-4.147	-2.900e-05	0.00741	1.247	2.057
trh_011_02030	CdLa ₂ NaNi ₆ Se ₅ Sn ₂ Tl ₃	20	-3.819	-4.288	1.000e-06	0.0082	1.865	1.319
trh_011_02453	BiLa ₂ Mn ₆ Sn ₉	18	-4.857	-5.575	0.000e+00	0.00938	1.545	0.877
trh_012_00842	Cs ₁₁ Tb ₆	17	-1.306	-1.627	-8.800e-05	0.00877	1.844	2.651
trh_012_01028	I ₈ Ni ₆ Sn	15	-2.984	-3.283	1.600e-05	0.00858	0.491	0.845
trh_012_01084	Bi ₈ La ₄ Ni ₇ Sn	20	-4.657	-4.957	-2.700e-05	0.00832	0.943	1.328
trh_012_01434	Br ₉ Co ₇ Cs ₂	18	-3.38	-3.766	8.000e-06	0.00617	1.391	1.14
trh_012_01643	Cs ₉ Dy ₆	15	-1.372	-1.724	2.000e-06	0.00353	2.812	4.051
trh_012_01709	Ni ₆ Sn ₂ Tl ₇	15	-3.144	-3.57	3.000e-06	0.00755	1.706	1.943
trh_012_01845	Cs ₃ I ₃ Ni ₆ Sn ₃	15	-3.204	-3.572	-3.000e-06	0.0085	1.494	2.22
trh_012_01894	La ₅ Ni ₈ Sn ₇	20	-4.702	-5.137	0.000e+00	0.00979	0.852	2.394
trh_012_02032	AlCo ₇ La ₁₀ Rh ₂	20	-5.632	-5.985	-1.000e-05	0.00788	0.992	2.178
trh_012_03159	Co ₇ I ₈ K	16	-3.337	-3.769	-5.500e-05	0.0076	1.236	1.099
trh_013_00084	I ₈ LiNi ₇	16	-3.051	-3.339	-2.000e-06	0.00848	1.061	1.295
trh_013_00977	Br ₈ PdRu ₆	15	-3.733	-4.75	-9.000e-06	0.00977	2.211	2.1
trh_013_01052	Br ₉ Co ₇ Cs ₂	18	-3.161	-3.827	-5.500e-05	0.00871	2.465	2.734
trh_013_01139	Co ₇ La ₁₀ Sn ₃	20	-5.408	-5.754	-2.000e-05	0.00997	1.282	2.613
trh_013_01330	Cs ₁₃ Ru ₆	19	-2.271	-2.807	-2.000e-06	0.00696	2.348	2.406
trh_013_01496	Br ₈ Co ₆ Cs ₂	16	-3.473	-3.774	-2.100e-05	0.00741	1.81	2.678
trh_013_01641	ClI ₆ Ni ₇	14	-3.108	-3.45	-2.000e-05	0.00792	1.181	1.151
trh_013_01775	KMn ₆ SbSn ₁₁	19	-4.468	-5.123	-8.000e-06	0.00803	1.197	1.937
trh_013_02680	Cl ₉ Mn ₆ Tl ₃	18	-3.896	-4.529	-9.000e-06	0.00845	1.002	0.721
trh_013_03260	Co ₇ La ₁₀ SbSn	19	-5.404	-5.773	0.000e+00	0.00842	1.141	1.571
trh_014_00134	I ₁₂ Ru ₆	18	-2.767	-3.881	-1.300e-05	0.00928	2.554	2.167
trh_014_00615	Co ₆ I ₈ La	15	-3.509	-3.929	-2.500e-05	0.00672	1.628	1.113

Table S13. The profile of generated materials with Truncated hexagonal lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
trh_014_00976	AlBr ₁₁ CoRu ₆	19	-3.661	-4.399	-6.000e-06	0.00927	1.15	3.272
trh_014_01337	Br ₂ Cl ₉ CsRu ₆	18	-3.655	-4.528	-3.100e-05	0.008	1.771	3.982
trh_014_02087	Cs ₉ Dy ₆	15	-1.321	-1.868	1.000e-06	0.00547	3.145	3.144
trh_014_02437	I ₁₀ Ni ₇ Y	18	-3.24	-3.548	-4.500e-05	0.00893	1.66	1.958
trh_014_03326	Co ₇ CsI ₈	16	-3.379	-3.719	1.700e-05	0.00769	1.281	1.196
trh_015_00332	Cs ₁₀ Tb ₆	16	-1.355	-1.685	-1.000e-06	0.0066	1.896	3.603
trh_015_00345	Br ₈ Cs ₂ Fe ₆	16	-3.678	-4.142	1.000e-06	0.00367	1.594	3.008
trh_015_00604	Fe ₆ I ₁₂	18	-3.178	-3.533	-1.100e-05	0.00359	1.446	1.813
trh_015_01221	I ₇ Ni ₆ Se	14	-3.004	-3.399	-1.100e-05	0.00659	0.779	1.473
trh_015_01236	Cs ₁₃ Dy ₆	19	-1.18	-1.55	-9.000e-06	0.00612	1.496	4.406
trh_015_01627	Ni ₆ Sn ₁₃	19	-3.943	-4.359	-1.000e-06	0.00627	1.014	1.758
trh_015_02140	CoNi ₇ SnTe ₁₀	19	-3.723	-4.298	-4.000e-06	0.00892	1.35	1.665
trh_015_02787	Fe ₆ I ₁₃ K	20	-3.048	-3.433	9.000e-06	0.00846	1.074	1.386
trh_015_03075	I ₈ Rb ₂ Ru ₆	16	-3.586	-4.314	-1.200e-05	0.00643	1.525	2.148
trh_015_03185	Cs ₉ Mn ₆	15	-2.764	-3.223	-1.000e-06	0.0095	2.377	2.559
trh_015_03311	Br ₇ ClCo ₆ Tl ₂	16	-3.36	-3.744	-9.000e-06	0.00919	1.345	1.418
trh_016_00077	BaCd ₂ Co ₆ La ₄ Sn ₇	20	-4.371	-4.777	-6.000e-06	0.00565	1.01	2.189
trh_016_00421	Cs ₈ MgYb ₆	15	-0.653	-0.959	-1.250e-04	0.00804	3.454	2.943
trh_016_00731	Cs ₄ Mn ₆ Te ₈	18	-4.021	-4.716	-1.700e-05	0.00953	1.405	1.491
trh_016_00887	Cs ₁₁ Dy ₆	17	-1.356	-1.616	-2.900e-05	0.00845	2.086	3.475
trh_016_00908	BrCl ₇ CsMn ₆ Rb	16	-4.162	-4.733	-1.400e-05	0.00612	1.867	3.688

Table S14. The profile of generated materials with Lieb lattice structures after DFT relaxation

Index	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
lieb_000_00012	Al ₂ Ba ₄ Nd ₃ SnSr	11	-3.047	-3.234	-1.000e-06	0.00558	1.118	2.173
lieb_000_00016	BiCaCeEuSnTb ₃	8	-3.896	-4.243	3.000e-06	0.00574	2.005	1.191
lieb_000_00036	Al ₂ Dy ₅ RhSr ₂ Zr	11	-4.228	-4.564	-2.800e-05	0.00524	0.725	2.164
lieb_000_00109	Ga ₄ Tb ₃ U	8	-4.322	-4.811	-3.000e-06	0.00562	0.748	0.75
lieb_000_00145	Ni ₆ PtZn	8	-5.078	-5.11	-3.300e-05	0.00322	0.188	0.117
lieb_000_00152	Fe ₅ Si ₂ TaTi ₄	12	-7.899	-8.125	0.000e+00	0.00688	0.679	0.561
lieb_000_00199	CaEuGd ₄ InSn	8	-3.77	-3.895	-5.000e-06	0.00394	1.445	2.306
lieb_000_00204	InMn ₃ ReRh ₂ V	8	-7.78	-8.036	-4.000e-06	0.00879	0.394	1.504
lieb_000_00215	Eu ₂ Gd ₃ In ₂ Nd	8	-3.18	-3.664	-2.000e-06	0.00584	1.282	1.7
lieb_000_00240	Ga ₃ Ru ₄ SeSn	9	-5.615	-5.895	-1.000e-06	0.00716	1.088	2.469
lieb_000_00253	Cs ₅ Nd ₃	8	-1.555	-1.823	-6.000e-06	0.00233	2.033	1.759
lieb_000_00254	CaPb ₄ Yb ₃	8	-2.766	-2.985	-1.000e-06	0.00463	0.677	1.348
lieb_000_00273	BiEu ₂ InNaTb ₃	8	-3.291	-3.447	3.000e-06	0.00913	1.294	1.739
lieb_000_00334	Ag ₃ Nd ₃ RbTe ₅	12	-3.666	-3.974	-1.000e-06	0.00585	0.762	3.011
lieb_000_00338	AlFe ₃ Pt ₄	8	-6.621	-6.697	-2.400e-05	0.00472	0.243	0.254
lieb_000_00356	Mn ₃ PS ₂ Si ₆	11	-6.457	-6.734	-3.000e-06	0.00541	0.374	0.518
lieb_000_00367	Br ₃ CaITb ₃	8	-2.686	-3.694	-5.000e-06	0.00485	2.14	2.742
lieb_000_00380	BaCaSnTl ₂ Yb ₃	8	-2.2	-2.411	7.000e-06	0.00524	1.012	0.545
lieb_000_00382	Bi ₂ Gd ₃ Na ₃	8	-3.306	-3.445	-2.000e-06	0.00494	2.128	1.596
lieb_000_00383	DyRu ₃ Se ₃ Tb	8	-6.188	-6.378	-3.000e-06	0.00886	0.576	0.623
lieb_000_00400	Al ₂ Fe ₃ Pd ₂ SrTb ₄	12	-5.092	-5.442	1.000e-05	0.00608	0.701	1.03
lieb_000_00406	Ba ₂ Gd ₃ HgTl ₂	8	-2.259	-2.907	-4.000e-06	0.00526	2.208	5.369
lieb_000_00407	Ga ₆ LaMgMn ₃	11	-4.477	-4.716	1.000e-06	0.00573	0.693	0.878
lieb_000_00414	AlCdDy ₃ Eu ₂ Mg	8	-2.856	-3.015	1.000e-06	0.00412	0.929	1.655
lieb_000_00425	Eu ₄ SnTb ₃	8	-3.115	-3.226	-1.000e-06	0.00361	1.548	4.493
lieb_000_00473	CeDy ₃ EuNa ₂ Sn	8	-3.403	-3.435	-6.000e-06	0.00553	0.724	0.402
lieb_000_00474	BaCdNa ₂ SnTb ₃	8	-2.553	-2.96	-4.000e-06	0.00439	1.592	2.395
lieb_000_00492	HCo ₃ DySm	6	-5.132	-5.762	-5.000e-06	0.00692	0.641	0.637
lieb_000_00510	Co ₉ FeNiV	12	-6.82	-7.08	1.000e-05	0.00948	0.376	0.395
lieb_000_00514	Fe ₃ Ni ₅	8	-6.302	-6.312	-1.000e-05	0.00521	0.091	0.054
lieb_000_00523	CoNi ₇ Ta ₄	12	-7.696	-7.863	-1.870e-04	0.00917	0.402	0.331
lieb_000_00533	Co ₆ PtZn	8	-5.896	-6.03	2.000e-06	0.0075	0.251	0.21
lieb_000_00540	PdSn ₅ Yb ₃	9	-2.851	-3.774	-2.000e-06	0.00638	2.451	3.778
lieb_000_00604	Ru ₃ Se ₂ Y ₂ Zr	8	-7.298	-7.525	0.000e+00	0.00517	0.72	0.858
lieb_000_00609	Al ₃ Co ₄ Fe ₂ Zn	10	-5.237	-5.779	-6.400e-05	0.00899	1.37	1.254
lieb_000_00632	AgBaSbSn ₂ SrYb ₃ Zn ₃	12	-2.242	-2.507	-1.000e-06	0.00474	1.385	2.238
lieb_000_00640	Co ₅ Pt ₃	8	-6.546	-6.557	1.000e-06	0.00684	0.081	0.059
lieb_000_00661	Ru ₄ Sn ₅ Sr ₂	11	-4.999	-5.474	-3.000e-06	0.00437	0.869	1.058
lieb_000_00701	Al ₃ MoNi ₇ Ta	12	-6.179	-6.315	-3.500e-05	0.0053	0.647	0.597
lieb_000_00711	Nd ₃ Sn ₅	8	-3.708	-4.756	-3.000e-06	0.00774	2.229	2.447
lieb_000_00726	GeMgRu ₃ Zn ₇	12	-3.272	-3.476	1.000e-06	0.00557	0.915	0.855
lieb_000_00732	CoGaGeNi ₄ Si	8	-5.387	-5.498	0.000e+00	0.00869	0.509	1.282
lieb_000_00748	Mn ₄ O ₇ V	12	-7.801	-8.069	-2.000e-06	0.00904	0.307	0.379
lieb_000_00782	Fe ₅ IrPRh	8	-7.71	-7.786	-5.000e-06	0.00507	0.157	0.269
lieb_000_00787	K ₄ SbSn ₃ Yb ₄	12	-2.435	-2.537	2.000e-06	0.00365	0.329	1.665
lieb_000_00849	CoFe ₃ Rh ₄	8	-7.161	-7.449	2.000e-06	0.00607	0.281	0.194
lieb_000_00860	GaNi ₇ Sn ₃ Zn	12	-4.467	-4.518	2.000e-06	0.00665	0.563	1.946
lieb_000_00867	EuGeLaNd ₃ Sb ₅	11	-4.642	-4.754	-7.000e-06	0.00252	0.824	0.552
lieb_000_00888	BaCsTl ₂ Yb ₃	7	-1.2	-1.742	1.000e-06	0.00326	1.959	4.551
lieb_000_00890	Ce ₅ Dy ₃ Ga ₄	12	-4.644	-4.872	1.900e-05	0.0049	1.14	0.656
lieb_000_00898	AgAs ₂ Nd ₃ SnSr	8	-4.095	-4.565	-5.000e-06	0.00353	1.532	2.682
lieb_000_00910	PbTb ₄ Tl ₃	8	-3.767	-3.837	-5.000e-06	0.00287	0.324	0.23

Table S14. The profile of generated materials with Lieb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
lieb_000_00922	CoGd ₃ GePdSn ₅	11	-4.475	-4.959	-2.000e-06	0.00505	0.569	1.959
lieb_000_00930	Co ₄ LaNi ₅ Sn	11	-5.641	-5.746	-7.000e-06	0.00842	0.41	0.367
lieb_000_00967	Cd ₄ Gd ₃ Se ₅	12	-3.368	-3.824	-3.000e-06	0.00343	0.787	1.703
lieb_000_00971	Fe ₅ Ni ₂ Os	8	-7.663	-7.738	-1.400e-05	0.00964	0.116	0.087
lieb_000_00982	Ca ₄ Ru ₃ Sn ₄	11	-4.937	-4.991	1.000e-06	0.00361	0.172	0.242
lieb_000_00994	Cs ₆ Gd ₃	9	-1.232	-1.699	-5.000e-06	0.00322	2.153	3.823
lieb_000_00998	CaDy ₆ MgRh ₄	12	-5.413	-5.499	-3.000e-06	0.0069	0.277	0.249
lieb_000_01033	Ni ₁₀ Zr ₂	12	-5.917	-6.19	-8.000e-06	0.00899	1.34	1.082
lieb_000_01042	Dy ₃ Ga ₅	8	-3.492	-4.101	0.000e+00	0.00936	0.668	2.197
lieb_000_01071	Br ₅ Dy ₃ Pb	9	-3.148	-4.074	-1.000e-06	0.00352	0.932	2.723
lieb_000_01089	Al ₂ Ga ₃ Ge ₂ LaRu ₃ Y	12	-5.065	-5.749	-2.000e-06	0.00757	0.935	1.001
lieb_000_01091	As ₅ I ₂ Ru ₄	11	-5.447	-5.697	5.000e-06	0.00954	0.67	1.689
lieb_000_01127	Fe ₈ Si ₄	12	-7.131	-7.404	7.000e-06	0.00682	1.339	1.593
lieb_000_01128	HGaMn ₃ NaSn ₂	8	-4.28	-4.974	0.000e+00	0.00793	0.728	2.738
lieb_000_01137	As ₄ CeCo ₅	10	-6.054	-6.331	1.000e-06	0.00709	0.911	2.575
lieb_000_01166	AlDy ₃ Se ₄ TeZn ₃	12	-3.353	-3.938	-3.000e-06	0.00377	1.061	2.829
lieb_000_01208	Dy ₃ IPbTe ₆	11	-3.989	-4.41	-8.000e-06	0.00815	1.423	3.494
lieb_000_01254	K ₄ MgP ₄ Tb ₃	12	-4.023	-4.088	-2.000e-06	0.00266	0.277	0.314
lieb_000_01267	Co ₂ FeNi ₅	8	-6.02	-6.039	-1.000e-05	0.00623	0.144	0.131
lieb_000_01279	KNa ₂ Nd ₃ Sb ₂	8	-2.782	-3.579	-3.900e-05	0.00895	2.322	2.763
lieb_000_01309	Ge ₉ Mn ₃	12	-5.317	-5.495	-1.000e-06	0.00643	0.753	0.717
lieb_000_01361	Au ₃ PdTl ₅ Yb ₃	12	-2.745	-2.924	0.000e+00	0.0098	1.42	1.596
lieb_000_01364	AsCl ₂ Gd ₃ I ₂ Rb	9	-3.008	-4.129	0.000e+00	0.00407	1.23	2.527
lieb_000_01383	CeLaSnTb ₃ Tl	7	-4.34	-4.519	-1.000e-06	0.00759	0.58	0.572
lieb_000_01418	Ag ₂ PrRu ₃ S ₄ Sm	11	-5.6	-5.942	0.000e+00	0.00267	0.397	0.477
lieb_000_01419	Gd ₃ Tl ₅	8	-3.259	-3.402	-3.000e-06	0.00368	0.317	0.234
lieb_000_01431	BrLiNdRu ₃ SSb	8	-5.344	-5.884	-1.000e-06	0.00536	1.112	1.296
lieb_000_01440	Nd ₄ Te ₄	8	-4.395	-5.341	-3.000e-06	0.00671	2.096	4.67
lieb_000_01523	Ni ₅ Pt ₂ Ti	8	-6.185	-6.238	1.000e-06	0.00457	0.245	0.283
lieb_000_01530	EuIn ₂ Tb ₄ Y	8	-4.072	-4.218	-1.000e-06	0.00527	0.373	1.05
lieb_000_01536	Gd ₃ SrTe ₄	8	-4.358	-4.901	0.000e+00	0.00518	1.499	1.343
lieb_000_01552	Co ₄ Dy ₈	12	-5.245	-5.486	-6.000e-06	0.00731	0.456	0.878
lieb_000_01597	As ₂ Cl ₄ CsYb ₃	10	-2.085	-3.607	-2.000e-06	0.00717	2.458	5.445
lieb_000_01602	Mn ₃ Ni ₉	12	-6.036	-6.296	0.000e+00	0.00619	0.45	0.504
lieb_000_01614	CaNa ₄ Nd ₃	8	-2.36	-2.426	2.000e-06	0.00561	1.285	1.525
lieb_000_01638	Co ₃ MnTe ₄	8	-5.272	-5.4	5.000e-06	0.00942	0.348	0.218
lieb_000_01641	Gd ₄ Na ₃ Tl	8	-2.85	-2.925	-1.600e-05	0.00696	1.676	3.294
lieb_000_01647	Ga ₅ Gd ₃ Ni ₄	12	-4.22	-4.66	1.000e-06	0.00618	1.617	2.422
lieb_000_01676	AlDy ₃ Mg ₇ Sn	12	-2.672	-2.757	-3.000e-06	0.00529	0.507	0.353
lieb_000_01709	BaEu ₂ In ₂ Yb ₃	8	-1.995	-2.117	1.000e-06	0.00544	1.301	5.307
lieb_000_01750	Mn ₃ Ni ₃ P ₃ SeV	11	-6.716	-6.817	2.000e-06	0.00752	0.293	0.249
lieb_000_01762	Al ₂ GeNi ₉	12	-5.225	-5.377	0.000e+00	0.00822	0.41	0.513
lieb_000_01765	AsCdCs ₂ IRu ₃ SnTe	10	-3.117	-4.544	1.000e-06	0.00357	1.427	1.222
lieb_000_01835	AgRb ₂ Se ₅ Tb ₃	11	-4.285	-4.559	-1.000e-06	0.00301	1.108	1.606
lieb_000_01881	AlFePtRu ₄ Ti	8	-8.014	-8.037	5.000e-06	0.00874	0.076	0.809
lieb_000_01933	AlAuNi ₇ V	10	-5.106	-5.589	-2.000e-06	0.00675	1.252	1.713
lieb_000_01949	Cs ₃ Nd ₃ RbSn	8	-1.477	-2.43	-2.200e-05	0.00694	4.415	8.116
lieb_000_01951	H ₄ Ni ₄ P ₂ Zn ₂	12	-3.615	-4.069	1.000e-06	0.00639	0.822	1.539
lieb_000_01986	AlAs ₂ Fe ₃ Na ₂	8	-4.587	-5.093	3.000e-06	0.00732	0.973	1.164
lieb_000_01994	AlErMg ₂ Mn ₅ NiRuTi	12	-6.03	-6.451	1.000e-06	0.00898	0.884	1.298
lieb_000_02026	Gd ₆ Sn ₂	8	-4.695	-4.843	0.000e+00	0.00403	0.496	0.299
lieb_000_02035	I ₈ Tb ₄	12	-3.576	-3.681	-4.000e-06	0.00562	0.65	0.68

Table S14. The profile of generated materials with Lieb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
lieb_000_02036	Hg ₄ Yb ₈	12	-1.349	-1.404	0.000e+00	0.0022	0.372	0.343
lieb_000_02153	Gd ₃ Tl ₅	8	-3.151	-3.406	-1.000e-06	0.00422	0.459	0.346
lieb_000_02155	Cs ₂ Gd ₃ S ₆ Sn	12	-4.886	-5.174	-1.000e-06	0.00618	0.722	1.475
lieb_000_02178	AsBr ₂ KNd ₃ RbSi ₂	10	-3.432	-4.251	-5.000e-06	0.00717	1.635	3.268
lieb_000_02179	GaNi ₆ Zn	8	-4.64	-4.799	-1.700e-05	0.00529	0.49	0.923
lieb_000_02195	As ₅ CeGeNi ₄ Sb	12	-5.043	-5.321	1.000e-06	0.00591	0.746	1.937
lieb_000_02235	AlMn ₃ Pt ₄	8	-6.956	-7.031	-3.000e-06	0.00668	0.203	1.465
lieb_000_02239	AgBrP ₄ Ru ₄ SnU	12	-6.452	-6.718	-2.000e-06	0.00795	0.454	0.741
lieb_000_02251	CoFeNi ₃ Pt ₃	8	-6.055	-6.135	-1.000e-06	0.00717	0.271	0.767
lieb_000_02324	Co ₄ Ni ₃ Pu	8	-7.035	-7.107	-2.500e-05	0.00955	0.22	0.826
lieb_000_02349	EuGd ₃ Tl ₄	8	-3.227	-3.309	-5.000e-06	0.00781	0.365	0.225
lieb_000_02358	Gd ₃ HfMnSe ₇	12	-5.251	-5.967	1.000e-05	0.0074	0.993	2.835
lieb_000_02410	AlDy ₅ LiOs ₄ Zr	12	-6.605	-6.852	-8.000e-06	0.00354	0.437	0.965
lieb_000_02454	I ₈ Yb ₄	12	-2.956	-3.169	-5.000e-06	0.00233	1.311	1.519
lieb_000_02468	Br ₈ FeTb ₃	12	-4.057	-4.256	0.000e+00	0.00529	0.358	1.125
lieb_000_02476	Ge ₆ Mn ₄ Nd	11	-6.243	-6.302	8.000e-06	0.00747	0.216	0.283
lieb_000_02500	Al ₄ CdDy ₄ Ga ₂ Tb	12	-3.671	-4.028	-1.000e-05	0.00469	1.489	2.803
lieb_000_02501	Co ₇ Pt	8	-6.728	-6.73	-7.000e-06	0.00709	0.028	0.02
lieb_000_02515	Fe ₄ Ga ₈	12	-4.651	-4.745	1.000e-06	0.00428	0.519	0.32
lieb_000_02523	Rb ₂ Se ₆ Tb ₃ Zr	12	-4.978	-5.113	-1.000e-05	0.008	0.684	0.708
lieb_000_02581	CaLaNd ₃ Pb ₂ Sr	8	-3.539	-3.995	-1.000e-06	0.00627	2.05	2.421
lieb_000_02645	Cd ₃ Gd ₃ Rb ₃ Sn ₃	12	-2.416	-2.691	-1.000e-06	0.00384	1.594	1.56
lieb_000_02728	Co ₈	8	-6.808	-6.841	-2.700e-05	0.00537	0.104	0.078
lieb_000_02740	BaBiBr ₂ EuSe ₃ Tb ₃	11	-3.95	-4.74	1.000e-06	0.00907	1.954	2.525
lieb_000_02745	Gd ₃ PdSn ₆ Tl ₂	12	-3.975	-4.176	-2.000e-06	0.00431	0.789	0.58
lieb_000_02788	Br ₄ Nd ₃ RbRe	9	-3.773	-4.427	-2.000e-06	0.00804	1.749	1.577
lieb_000_02813	AuBaCdDy ₃ GeHoInLaSb ₂	12	-3.896	-4.263	-2.000e-06	0.00611	0.426	2.348
lieb_000_02818	Mn ₃ Se ₃	6	-5.411	-6.09	-6.900e-05	0.00629	1.572	0.772
lieb_000_02837	Co ₄ Pt ₄	8	-6.411	-6.44	-9.000e-06	0.0073	0.152	0.766
lieb_000_02851	As ₂ GaNi ₄ P	8	-4.811	-5.116	0.000e+00	0.00753	0.87	1.615
lieb_000_02855	Fe ₃ NiTe ₄	8	-5.274	-5.38	-1.000e-06	0.00799	0.373	0.341
lieb_000_02866	Ge ₄ La ₄ RhRu ₃	12	-6.688	-6.779	0.000e+00	0.00612	0.296	0.276
lieb_000_02883	Na ₃ Nd ₃ Sn ₂	8	-2.949	-3.487	0.000e+00	0.004	1.412	1.728
lieb_000_02884	EuTb ₃ Tl ₄	8	-3.006	-3.296	-2.000e-06	0.00359	0.613	0.589
lieb_000_02896	Al ₅ BiDy ₅ Tl	12	-4.03	-4.026	-2.000e-06	0.00518	0.23	0.297
lieb_000_02903	Mg ₄ Mn ₃ PtSi ₃ Zn	12	-4.493	-4.85	0.000e+00	0.00752	0.572	1.82
lieb_000_02909	AlCoNi ₉	11	-5.113	-5.425	-2.000e-06	0.00695	0.64	0.489
lieb_000_02932	Na ₂ Nd ₄ SnSr	8	-3.31	-3.315	-4.000e-06	0.00607	0.273	0.139
lieb_000_02991	La ₂ Ni ₃ Sn ₂	7	-5.041	-5.321	-3.000e-06	0.0055	0.397	1.96
lieb_000_02998	BaDy ₃ Na ₄	8	-2.215	-2.295	1.000e-06	0.00338	1.403	2.475
lieb_000_03059	Cd ₃ Dy ₃ NaPTe ₄	12	-3.288	-3.61	-1.000e-06	0.0058	1.511	1.862
lieb_000_03066	EuNd ₄ Tl ₃	8	-3.53	-3.705	-3.000e-06	0.0038	0.582	0.307
lieb_000_03090	CdRb ₄ Sn ₄ Tb ₃	12	-3.017	-3.104	0.000e+00	0.00538	0.475	0.405
lieb_000_03100	GaRu ₃ SbSiTmU	8	-6.853	-7.327	-1.000e-06	0.00347	1.523	0.846
lieb_000_03103	AgBiGd ₃ GeSb ₂ Se ₂	10	-4.125	-4.698	-8.000e-06	0.00684	1.802	2.222
lieb_000_03115	Cd ₃ Ru ₇ SnZn	12	-5.438	-5.774	0.000e+00	0.00633	1.085	1.607
lieb_000_03149	Gd ₄ Rb ₂ S ₄ Sr ₂	12	-4.118	-4.356	-1.000e-06	0.00244	0.254	1.364
lieb_000_03199	Gd ₄ NaSn ₃	8	-3.473	-4.294	-1.900e-05	0.00814	1.982	5.541
lieb_000_03217	Gd ₄ RhSeSi ₃ Sr ₃	12	-4.323	-4.766	-3.000e-06	0.00496	1.429	2.124
lieb_000_03229	CoFeLiNi ₄ PSi ₂ VZn	12	-5.308	-5.61	-2.000e-06	0.00637	0.851	1.927
lieb_000_03251	Br ₂ Gd ₃ NaTl ₂	8	-2.877	-3.56	-3.000e-06	0.00275	1.362	2.14
lieb_000_03274	Ge ₂ NaRu ₃ Y	7	-5.738	-6.398	0.000e+00	0.00629	1.828	1.614

Table S14. The profile of generated materials with Lieb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
lieb_000_03281	Ru ₄ S ₈	12	-5.206	-5.902	6.000e-06	0.00574	0.638	0.695
lieb_000_03298	Ag ₄ Ge ₂ PrSnTb ₃	11	-3.858	-4.139	-8.000e-06	0.00631	0.548	2.194
lieb_000_03346	Na ₃ Ru ₃ Sn ₂	8	-4.251	-4.511	-1.000e-06	0.00566	1.107	1.519
lieb_000_03356	Tb ₃ Tl ₅	8	-2.951	-3.391	-4.000e-06	0.0039	0.761	2.204
lieb_000_03357	Dy ₃ EuSn ₃ Sr	8	-3.463	-3.999	0.000e+00	0.0073	1.446	3.017
lieb_000_03360	As ₄ Nd ₃ Rb ₄ Sn	12	-3.892	-3.987	3.000e-06	0.00478	0.702	0.614
lieb_000_03389	Br ₅ CaGdTb ₃	10	-3.335	-3.919	-1.000e-06	0.00261	1.423	2.261
lieb_000_03444	Ce ₂ Co ₄ Ga ₅ Ge	12	-4.986	-5.262	-1.000e-06	0.00692	0.919	2.045
lieb_000_03454	Al ₂ Ca ₅ Gd ₃ SnTl	12	-3.184	-3.246	-1.000e-06	0.00343	0.277	0.504
lieb_000_03502	BiBr ₂ Eu ₂ PtTb ₃	9	-3.437	-4.364	-1.000e-06	0.00683	1.079	2.105
lieb_000_03521	Ni ₁₀ ScTa	12	-6.114	-6.23	-6.000e-06	0.00724	0.381	0.362
lieb_000_03563	Cl ₄ Dy ₃ KRe	9	-3.694	-4.511	-2.300e-05	0.00805	2.111	3.346
lieb_000_03572	Ga ₇ Ru ₃ Sr ₂	12	-4.16	-4.534	0.000e+00	0.00425	0.9	1.21
lieb_000_03595	Fe ₄ Se ₄	8	-5.83	-6.153	-9.000e-06	0.00672	0.423	0.245
lieb_000_03602	DyFe ₄ Te ₃	8	-5.413	-5.791	1.000e-06	0.00723	0.597	0.45
lieb_000_03619	Nd ₄ Se ₈	12	-5.196	-5.314	-3.000e-06	0.00403	0.307	0.329
lieb_000_03649	CaCdDy ₃ NaTl ₂	8	-2.207	-2.96	0.000e+00	0.00397	2.514	2.583
lieb_000_03652	Nd ₆ Sn ₂	8	-4.74	-4.793	-2.000e-06	0.00316	0.202	0.223
lieb_000_03715	CdDy ₄ NaSb ₂	8	-3.299	-3.999	0.000e+00	0.00357	1.711	2.855
lieb_000_03725	CdDy ₅ Pt ₄ Sb ₂	12	-4.879	-5.612	-1.000e-06	0.00524	1.258	1.262
lieb_000_03761	GaGd ₃ Na ₂ Sn ₂	8	-3.433	-3.646	1.000e-06	0.00656	0.632	0.319
lieb_000_03769	AlCa ₂ GaTb ₃ Tl	8	-3.116	-3.523	0.000e+00	0.00715	1.67	3.015
lieb_000_03777	Ni ₅ ThYb	7	-5.128	-5.33	-2.300e-05	0.00993	0.874	1.286
lieb_000_03811	NaTl ₄ Yb ₃	8	-1.882	-2.102	-1.000e-06	0.00345	0.535	1.579
lieb_000_03818	Ge ₈ Ru ₄	12	-6.052	-6.25	0.000e+00	0.00525	0.394	1.108
lieb_000_03826	AlCoFe ₆	8	-7.331	-7.427	-5.000e-06	0.0056	0.177	0.135
lieb_000_03832	AsCl ₄ CsDy ₃	9	-2.886	-4.355	-3.000e-06	0.00774	2.108	2.025
lieb_000_03870	Cu ₂ ErFe ₃ NbNi ₂ TaVZr	12	-6.839	-7.231	-3.000e-06	0.00329	1.168	1.098
lieb_000_03880	BrRb ₂ Sn ₂ Tb ₃ Te ₄	12	-3.751	-4.1	-1.500e-05	0.00785	0.871	2.125
lieb_000_03937	Ge ₂ Ni ₆	8	-5.441	-5.526	0.000e+00	0.00763	0.218	0.195
lieb_000_03940	Dy ₃ Na ₅	8	-2.138	-2.215	2.000e-06	0.00677	1.338	1.681
lieb_000_03986	Cl ₃ Dy ₃ IKSb	9	-2.352	-4.12	-1.000e-06	0.00765	2.564	3.533
lieb_000_03991	Co ₈ Li ₂ Ti	11	-5.758	-5.996	-4.000e-06	0.00662	0.505	0.566
lieb_000_04007	Co ₄ EuNaS ₄	10	-5.38	-5.44	1.400e-05	0.00891	0.183	0.107
lieb_000_04025	Al ₂ GaNi ₇ U ₂	12	-5.752	-6.205	-3.000e-06	0.00858	1.488	1.568
lieb_000_04061	Mn ₄ Ni ₈	12	-6.475	-6.587	-8.000e-06	0.00724	0.275	0.157
lieb_000_04096	AsCo ₃ HfLiSSe	8	-5.687	-5.955	-2.000e-06	0.00993	0.899	1.379
lieb_000_04105	Ni ₃ S ₃ Y	7	-5.226	-5.803	-1.000e-06	0.00861	0.997	1.114
lieb_000_04123	Dy ₃ Eu ₂ Sn ₂ Sr	8	-3.464	-3.656	-1.000e-06	0.006	1.843	2.019
lieb_000_04136	Bi ₄ Yb ₈	12	-2.884	-2.917	9.000e-06	0.00359	0.276	0.233
lieb_000_04143	AuGaNi ₅ Sb	8	-4.685	-4.818	0.000e+00	0.00708	1.414	3.762
lieb_000_04150	Cs ₂ PbYb ₃	6	-1.275	-1.599	-2.000e-07	0.00626	1.225	1.156
lieb_000_04153	Dy ₃ MgRb ₄ Sn ₄	12	-2.89	-3.01	1.000e-06	0.00516	1.02	1.031
lieb_000_04164	As ₄ Ni ₅ VZn	11	-4.931	-5.233	-1.000e-06	0.0081	0.929	1.59
lieb_000_04165	Co ₄ Ni ₃ Zn	8	-5.569	-5.586	4.000e-06	0.00526	0.075	1.31
lieb_000_04168	Fe ₄ Pt ₆ Si ₂	12	-6.456	-6.788	-8.000e-06	0.00968	0.809	0.547
lieb_000_04217	GeNi ₇	8	-5.326	-5.469	-2.200e-05	0.00428	0.204	0.167
lieb_000_04229	Co ₃ SSe ₂	6	-4.7	-5.61	-3.200e-05	0.00806	1.238	1.525
lieb_000_04237	La ₂ Sn ₂ Tb ₃	7	-4.57	-4.774	-7.000e-06	0.00567	1.711	2.438
lieb_000_04248	GaNd ₅ Tl ₂	8	-3.841	-4.133	-5.000e-06	0.00427	0.738	1.317
lieb_000_04287	AuGeLa ₂ Ni ₄ Sn ₃	11	-4.747	-4.987	-2.000e-06	0.00633	0.472	0.631
lieb_000_04309	AlCo ₄ GeLa ₂	8	-5.394	-6.044	-1.100e-05	0.00909	1.184	1.22

Table S14. The profile of generated materials with Lieb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
lieb_000_04325	AlScSn ₃ Tb ₃	8	-4.575	-4.813	-5.000e-06	0.00911	0.548	0.595
lieb_000_04349	LiNi ₄ PSe ₃	9	-4.369	-4.723	-4.000e-06	0.00649	0.596	1.012
lieb_000_04381	Cs ₄ RbYb ₃	8	-0.583	-0.922	1.800e-06	0.00329	3.289	5.516
lieb_000_04453	Fe ₃ NaSe ₃ Y	8	-5.133	-5.534	-3.000e-06	0.00767	1.135	1.952
lieb_000_04488	Ba ₂ Gd ₃ Sb ₃	8	-3.772	-4.362	1.000e-06	0.00538	0.999	3.358
lieb_000_04494	Pt ₄ Ru ₃ U	8	-7.975	-8.118	-3.000e-06	0.00528	0.386	0.458
lieb_000_04503	BaRh ₃ Sn ₃ Tb ₃ Zn	11	-4.473	-5.026	-4.000e-06	0.00619	1.401	1.091
lieb_000_04527	AgCe ₂ Co ₃ S ₄	10	-5.917	-6.033	-7.100e-05	0.0085	0.213	0.325
lieb_000_04620	Ag ₃ Ru ₄ Sn ₅	12	-4.613	-5.242	-5.000e-06	0.0095	0.26	1.615
lieb_000_04646	Ni ₇ Zn	8	-4.906	-4.966	8.000e-06	0.00659	0.168	0.18
lieb_000_04658	Br ₄ SiTb ₃ Te	9	-3.488	-4.414	-1.000e-06	0.00354	2.404	2.965
lieb_000_04664	Ni ₆ Pt ₂	8	-5.606	-5.665	5.000e-06	0.00557	0.265	0.302
lieb_000_04686	Fe ₅ Ni ₂ U	8	-7.8	-7.838	-3.000e-06	0.00585	0.186	0.122
lieb_000_04716	Ca ₅ Dy ₃ Ni ₄	12	-3.743	-3.889	-1.000e-05	0.00424	0.972	0.455
lieb_000_04718	EuInLuNd ₄ Sn	8	-4.207	-4.3	1.000e-06	0.00734	0.274	0.321
lieb_000_04730	AlBr ₂ Sn ₂ Tb ₃ Ti ₂	10	-4.185	-4.81	-4.000e-06	0.005	1.783	3.749
lieb_000_04816	LiMn ₃ Pt ₄	8	-6.369	-6.696	-1.000e-06	0.00879	0.435	1.512
lieb_000_04828	Co ₇ Ge	8	-6.595	-6.642	1.000e-06	0.00448	0.1	0.102
lieb_000_04850	AlFe ₃ GaMnPtSi	8	-6.178	-6.63	-3.000e-06	0.00829	0.708	1.717
lieb_000_04890	GeNi ₆ Tc	8	-5.849	-5.985	-4.000e-06	0.00656	0.378	0.31
lieb_000_04895	Eu ₂ NaNd ₃ SnSr	8	-2.799	-3.16	-2.000e-06	0.00635	1.38	1.743
lieb_000_04951	Dy ₃ EuInPbSnTl	8	-3.361	-3.828	-3.000e-06	0.00576	1.571	1.698
lieb_000_04960	Ga ₃ GeNdRu ₃	8	-5.561	-5.808	-5.000e-06	0.00976	1.221	2.215
lieb_000_04965	Gd ₃ LuTl ₄	8	-3.455	-3.631	-1.000e-05	0.00999	0.459	1.651
lieb_000_04975	Co ₃ Se ₅ Tl	9	-4.293	-4.698	-1.300e-05	0.00722	0.8	1.572
lieb_000_04982	Ni ₉ ScYb	11	-4.93	-5.243	-4.000e-06	0.00806	0.4	1.882
lieb_000_04994	AlEuNaSnTb ₄	8	-3.58	-3.822	0.000e+00	0.00621	1.71	3.367
lieb_000_05003	Ca ₂ GeNi ₃ Zn	7	-3.573	-3.953	-1.000e-06	0.00562	0.711	1.297
lieb_000_05012	Ga ₂ GeK ₂ NaRu ₃ Te ₃	12	-3.776	-4.447	-1.000e-05	0.00764	1.548	1.674
lieb_000_05080	Nd ₄ Tl ₄	8	-3.594	-3.743	1.000e-06	0.00285	0.418	0.304
lieb_000_05091	Eu ₄ Ru ₄ S ₄	12	-5.791	-5.864	-4.000e-06	0.0048	0.53	0.484
lieb_000_05131	Br ₂ LiNd ₃ Te ₄	10	-4.065	-4.454	0.000e+00	0.0082	1.15	2.155
lieb_000_05143	Gd ₃ Sn ₄ Sr ₅	12	-3.489	-3.583	3.000e-06	0.00467	0.359	0.334
lieb_000_05152	Al ₉ Ru ₃	12	-4.894	-5.406	-1.000e-06	0.00704	1.061	0.981
lieb_000_05177	CoNd ₃ S ₅ Sn ₃	12	-4.064	-5.436	-1.200e-05	0.00764	1.917	1.915
lieb_000_05190	Ni ₈	8	-5.338	-5.407	0.000e+00	0.00498	0.138	0.804
lieb_000_05242	Ni ₇ V	8	-5.849	-5.989	-2.000e-05	0.00477	0.279	0.266
lieb_000_05291	CaGa ₄ Gd ₄ Sr ₃	12	-3.155	-3.304	1.000e-06	0.0035	0.748	3.041
lieb_000_05343	CdCl ₈ Ru ₃	12	-3.339	-3.937	2.000e-06	0.00607	1.273	0.914
lieb_000_05361	AlFe ₃ GaSi ₂ Tc	8	-6.506	-6.705	0.000e+00	0.00578	0.7	0.791
lieb_000_05402	AlDy ₃ EuInNaSn	8	-3.715	-3.689	-1.000e-06	0.00447	0.685	1.605
lieb_000_05409	Ge ₄ Ni ₄	8	-4.882	-5.179	-8.000e-06	0.00693	0.782	0.866
lieb_000_05452	ISnTb ₃ Tl ₂	7	-3.389	-3.645	-7.000e-06	0.0073	0.882	0.821
lieb_000_05484	CeDy ₅ NdYb	8	-4.256	-4.27	-7.000e-06	0.00399	0.143	0.109
lieb_000_05485	EuIn ₂ La ₂ Ru ₃	8	-5.129	-5.677	-2.200e-05	0.00907	0.925	1.749
lieb_000_05496	Co ₂ GaMn ₅	8	-7.436	-7.647	-2.000e-06	0.00731	0.209	0.201
lieb_000_05526	Al ₃ Ca ₅ SnYb ₃	12	-2.511	-2.552	-1.000e-06	0.00845	0.227	0.443
lieb_000_05533	Cl ₄ Gd ₃ RbSb	9	-2.995	-4.288	-1.000e-06	0.00245	1.478	1.802
lieb_000_05558	Al ₃ Co ₆ TmV	11	-6.026	-6.252	-5.000e-06	0.00576	0.444	0.638
lieb_000_05580	Fe ₃ Ni ₅	8	-6.175	-6.315	2.000e-06	0.00686	0.194	0.249
lieb_000_05651	GePt ₄ Ru ₃	8	-7.023	-7.057	1.000e-06	0.00591	0.172	0.752
lieb_000_05713	AsGd ₄ K ₄ Sb ₃	12	-3.918	-3.963	7.000e-06	0.0083	0.313	0.262

Table S14. The profile of generated materials with Lieb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
lieb_000_05753	EuGd ₃ KPSnSr	8	-3.513	-3.74	0.000e+00	0.00498	0.957	3.472
lieb_000_05773	P ₄ Rb ₄ Ru ₄	12	-5.029	-5.272	-1.000e-06	0.00588	0.493	0.521
lieb_000_05814	Co ₃ LiMnSe ₃	8	-4.877	-5.307	2.000e-06	0.00902	0.516	0.628
lieb_000_05831	CaGePSnYb ₅	9	-2.809	-3.117	1.000e-06	0.005	0.73	0.418
lieb_000_05836	HgK ₄ Nd ₃ Sn ₄	12	-3.072	-3.117	-2.000e-06	0.00677	0.135	1.592
lieb_000_05848	ErGa ₈ Ru ₃	12	-4.612	-4.859	-1.000e-06	0.00717	0.735	0.726
lieb_000_05855	AlBi ₄ GeRu ₃	9	-5.208	-5.497	-1.000e-06	0.00822	0.9	1.922
lieb_000_05859	Dy ₃ K ₂ Tl ₃	8	-2.333	-2.752	-3.000e-06	0.00542	2.006	3.775
lieb_000_05886	AuGa ₃ GeNd ₃ Rb ₄	12	-2.803	-3.025	-1.800e-05	0.00949	1.782	2.696
lieb_000_05890	CuMn ₃ S ₄	8	-6.062	-6.354	-1.100e-05	0.00808	0.458	0.421
lieb_000_05921	Ga ₂ K ₅ Yb ₃	10	-1.382	-1.489	9.000e-06	0.00587	1.694	1.425
lieb_000_05978	Ga ₃ Mn ₄	7	-6.041	-6.232	6.000e-06	0.00573	0.657	1.076
lieb_000_06004	As ₂ P ₂ Rb ₄ Tb ₃	11	-4.061	-4.126	-2.000e-06	0.00634	0.185	0.342
lieb_000_06031	AlNi ₁₀ Ti	12	-5.598	-5.775	-4.000e-06	0.00448	0.365	0.209
lieb_000_06049	Cs ₄ Dy ₃ Pb	8	-1.945	-2.357	-4.400e-05	0.00818	1.714	2.178
lieb_000_06096	Al ₃ Eu ₃ In ₃ Tb ₃	11	-3.032	-3.278	-1.400e-05	0.00904	1.313	1.305
lieb_000_06110	Sn ₃ Yb ₉	12	-2.347	-2.422	0.000e+00	0.00281	0.447	0.353
lieb_000_06111	Cd ₄ PdRu ₃	8	-3.229	-4.247	1.000e-06	0.00985	1.601	1.525
lieb_000_06162	Rh ₄ Sn ₅ Tb ₃	12	-5.097	-5.752	0.000e+00	0.00478	0.932	1.813
lieb_000_06164	AlNi ₈ Ru ₃	12	-5.849	-6.305	1.100e-05	0.00884	0.815	1.009
lieb_000_06176	Bi ₂ EuIn ₆ Yb ₃	12	-2.563	-2.84	0.000e+00	0.00593	1.025	0.708
lieb_000_06203	AsCdGd ₃ ISbSeSr	9	-3.549	-4.313	1.000e-06	0.00453	1.881	2.613
lieb_000_06218	Co ₆ GePd	8	-6.319	-6.357	-8.000e-06	0.00891	0.117	0.125
lieb_000_06246	Co ₅ Fe ₃	8	-7.138	-7.307	-1.000e-06	0.0042	0.178	0.241
lieb_000_06293	NbNi ₁₀ V	12	-6.21	-6.271	1.000e-06	0.00681	0.187	0.262
lieb_000_06343	AlGa ₂ Ni ₅	8	-4.881	-5.007	-1.500e-05	0.00555	0.467	0.385
lieb_000_06344	Co ₄ GaMn ₂ Rh	8	-6.908	-6.972	-1.000e-06	0.00731	0.163	0.766
lieb_000_06372	Cs ₆ Dy ₃	9	-1.462	-1.65	-1.000e-06	0.00323	1.506	1.726
lieb_000_06376	Dy ₃ NaTl ₄	8	-3.059	-3.137	-1.000e-06	0.0058	0.276	0.294
lieb_000_06383	Ni ₄ Tb ₈	12	-4.859	-5.089	-1.000e-06	0.00626	0.686	1.774
lieb_000_06387	Al ₆ BaLaMn ₃	11	-4.923	-5.208	0.000e+00	0.00269	0.396	0.737
lieb_000_06405	Cl ₄ CsDy ₃ Ir	9	-3.613	-4.616	-2.000e-06	0.00511	1.756	4.03
lieb_000_06406	Br ₃ Gd ₃ NaSn	8	-3.118	-3.977	-1.000e-06	0.0034	1.457	2.518
lieb_000_06435	Cr ₂ Ni ₅ W	8	-7.104	-7.341	-1.300e-05	0.00946	0.365	0.209
lieb_000_06443	Ca ₂ Sn ₄ Yb ₆	12	-2.766	-2.807	-3.000e-06	0.00319	0.276	0.423
lieb_000_06506	Dy ₆ GaTh	8	-4.685	-4.731	2.000e-06	0.0058	0.194	1.024
lieb_000_06537	AlMn ₄ NbNiRe	8	-8.348	-8.455	-2.000e-06	0.00756	0.926	1.128
lieb_000_06552	Fe ₂ GaGd ₃ PSn ₃ Te ₂	12	-4.351	-5.012	0.000e+00	0.00892	1.016	1.626
lieb_000_06583	Fe ₂ Ga ₆ Mn ₄	12	-5.467	-5.712	-3.000e-06	0.00546	0.596	0.57
lieb_000_06590	FeNi ₃ P ₇	11	-5.288	-5.803	-1.000e-06	0.00628	0.874	0.928
lieb_000_06591	EuGa ₃ Gd ₄	8	-3.72	-3.923	-6.000e-06	0.00725	0.547	0.391
lieb_000_06610	Sn ₈ Tb ₃ Tl	12	-4.07	-4.187	-2.000e-06	0.00589	0.364	0.336
lieb_000_06643	As ₃ Ge ₂ Ni ₃ Pt ₃ Sc	12	-5.503	-5.686	8.000e-06	0.00465	0.552	0.674
lieb_000_06646	LaNa ₄ Tb ₃	8	-2.607	-2.666	-2.000e-06	0.00449	1.272	0.576
lieb_000_06650	AlBiEu ₂ Nd ₃ Sr	8	-3.18	-3.61	0.000e+00	0.00816	1.993	2.71
lieb_000_06669	CaI ₇ Nd ₃	11	-3.115	-3.617	-3.000e-06	0.00468	1.492	1.743
lieb_000_06677	Br ₃ CaTb ₃ Tl	8	-2.965	-3.68	0.000e+00	0.00473	1.887	3.912
lieb_000_06729	Ga ₇ Ni ₅	12	-4.073	-4.19	-1.000e-06	0.00702	0.186	0.211
lieb_000_06752	Mn ₅ Si ₃ Sn ₂	10	-6.243	-6.784	-1.400e-05	0.00731	1.375	2.218
lieb_000_06758	Al ₂ CdCu ₂ GaMn ₄ NiTa	12	-5.541	-5.849	-3.000e-06	0.00647	0.71	0.507
lieb_000_06767	Co ₄ FeGa ₂ Ti	8	-6.327	-6.417	7.000e-06	0.00299	0.791	1.597
lieb_000_06778	CoLu ₄ Ni ₅ Si ₂	12	-5.032	-5.908	1.700e-05	0.00892	0.947	0.924

Table S14. The profile of generated materials with Lieb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
lieb_000_06781	Al ₄ Ca ₄ Ni ₄	12	-3.908	-4.082	-1.000e-06	0.00574	0.431	0.283
lieb_000_06820	Mn ₄ S ₄	8	-6.48	-7.038	-4.000e-06	0.00606	0.69	0.559
lieb_000_06822	Ba ₂ Cd ₂ CsNd ₃ Sb ₄	12	-3.442	-3.696	-2.800e-05	0.00555	0.603	0.984
lieb_000_06831	CaDy ₅ LuPt ₃ Sb	11	-4.999	-5.451	-2.000e-06	0.00866	1.115	1.752
lieb_000_06854	CuLa ₂ Ni ₃ PtSe ₄	11	-4.761	-5.25	0.000e+00	0.00669	1.241	1.352
lieb_000_06867	BaGd ₃ SnSrTl	7	-3.104	-3.545	-1.200e-05	0.00759	2.128	2.808
lieb_000_06892	Na ₄ Nd ₃ Sn	8	-2.737	-2.866	0.000e+00	0.00351	0.724	0.803
lieb_000_06894	AgGe ₂ Nd ₃ SnTe ₅	12	-3.813	-4.451	-1.300e-05	0.00693	2.161	2.288
lieb_000_06911	Ba ₂ EuGd ₄ NaSn ₃ Tl	12	-3.392	-3.538	1.000e-06	0.00745	1.127	0.714
lieb_000_06933	InTe ₄ Yb ₃	8	-3.408	-3.733	5.000e-06	0.00397	1.536	2.867
lieb_000_06947	Co ₃ GaPr ₂ SbSn ₃	10	-4.864	-5.265	3.000e-06	0.00786	0.82	2.67
lieb_000_06962	La ₂ Ru ₃ SnTe ₂	8	-5.632	-6.283	-1.000e-06	0.00919	0.831	1.87
lieb_000_06964	Ga ₂ Ni ₄ RuV	8	-5.856	-5.891	-1.000e-06	0.00563	0.182	0.81
lieb_000_06966	Co ₃ Ge ₂ Mg ₂ Si ₅	12	-4.772	-5.103	-1.000e-06	0.00723	0.267	0.52
lieb_000_07000	Bi ₅ Dy ₅ Sb	11	-4.472	-4.865	1.000e-06	0.00462	1.546	1.328
lieb_000_07065	Pd ₅ Ru ₃	8	-6.409	-6.489	-3.000e-06	0.00319	0.13	0.098
lieb_000_07071	Ru ₃ Sn ₆ U ₂	11	-6.372	-6.741	3.000e-06	0.00367	1.029	1.454
lieb_000_07137	Br ₅ Gd ₂ Tb ₃	10	-3.442	-4.077	-2.400e-05	0.00698	1.45	3.006
lieb_000_07144	CoFe ₇	8	-7.822	-7.927	-1.100e-05	0.00419	0.2	0.14
lieb_000_07235	Ba ₂ EuGdSnTb ₃	8	-3.371	-3.487	-1.000e-06	0.00385	1.996	1.069
lieb_000_07241	Gd ₃ In ₃ Na ₂	8	-3.151	-3.167	-1.000e-06	0.00347	0.57	1.992
lieb_000_07253	Tl ₃ Yb ₅	8	-1.842	-2.099	1.000e-06	0.00203	1.523	0.567
lieb_000_07263	GaNi ₆ Zr	8	-5.682	-5.815	-7.000e-06	0.00496	1.269	2.47
lieb_000_07267	BiEuLaSn ₂ Tb ₃	8	-4.074	-4.506	-2.000e-06	0.00509	0.814	0.531
lieb_000_07315	Ni ₇ Ta	8	-6.384	-6.388	4.000e-06	0.00719	0.052	0.031
lieb_000_07329	GdNaSnTb ₄	7	-3.784	-3.995	-2.000e-06	0.00387	0.581	3.204
lieb_000_07334	Na ₃ Tb ₃ Tl ₂	8	-2.349	-2.781	0.000e+00	0.0066	1.91	2.279
lieb_000_07337	Pd ₄ PtRu ₃	8	-6.009	-6.642	-1.000e-06	0.00375	0.465	0.276
lieb_000_07361	La ₄ MgPd ₄ Ru ₃	12	-5.73	-6.066	-8.000e-06	0.00473	0.564	1.812
lieb_000_07374	Dy ₃ La ₂ Sn ₃	8	-4.688	-4.884	1.000e-06	0.00659	0.494	0.419
lieb_000_07381	BiCaEuSn ₂ Tb ₃	8	-3.518	-4.076	3.000e-06	0.00817	1.992	1.32
lieb_000_07407	Cd ₂ Co ₃ HoP ₅	11	-5.044	-5.234	-2.100e-05	0.00974	0.62	0.601
lieb_000_07412	GaGd ₃ LaNaPb	7	-3.737	-3.948	0.000e+00	0.00746	0.308	1.719
lieb_000_07446	Co ₂ Ge ₃ LaTb ₄	10	-5.188	-5.488	1.000e-06	0.00888	0.846	0.905
lieb_000_07448	Ge ₂ InYb ₈ Zn	12	-2.439	-2.385	0.000e+00	0.00257	0.465	0.538
lieb_000_07459	Dy ₃ Na ₂ PbSr ₂	8	-2.463	-2.828	0.000e+00	0.00177	1.45	1.077
lieb_000_07468	Co ₇ Ga ₃ MnSi	12	-5.54	-6.121	2.000e-06	0.0068	0.929	1.077
lieb_000_07500	Ce ₂ Co ₃	5	-6.476	-6.864	0.000e+00	0.00835	0.624	0.797
lieb_000_07540	AlCo ₇	8	-6.519	-6.617	-1.400e-04	0.00701	0.229	0.14
lieb_000_07563	BeFe ₄ Li ₂ MnP ₃	11	-5.701	-6.239	-4.000e-06	0.00865	1.052	1.811
lieb_000_07593	BaCs ₃ Dy ₃ Sb ₃	10	-3.134	-3.457	-2.000e-06	0.00278	0.911	1.091
lieb_000_07599	GeLa ₂ SnYb ₆ Zn ₂	12	-2.645	-2.719	-4.000e-06	0.00598	0.552	0.312
lieb_000_07601	Dy ₆ Tl ₂	8	-3.957	-4.046	0.000e+00	0.00173	0.569	1.186
lieb_000_07658	Cl ₄ KSbYb ₃	9	-2.575	-3.697	-4.000e-06	0.00382	1.981	2.901
lieb_000_07683	Pt ₅ Ru ₃	8	-7.073	-7.209	-2.000e-06	0.00534	0.153	0.208
lieb_000_07691	Gd ₄ Sn ₄	8	-3.903	-4.779	-1.000e-05	0.00849	1.906	2.597
lieb_000_07704	I ₄ Ru ₄	8	-4.65	-4.852	-2.000e-06	0.00838	0.425	0.36
lieb_000_07721	Al ₂ Fe ₆	8	-6.852	-7.075	-1.600e-05	0.00581	0.246	0.226
lieb_000_07751	Co ₄ Ni ₅ UV ₂	12	-6.986	-7.167	2.000e-06	0.00668	0.436	0.459
lieb_000_07757	Br ₅ PdRu ₃ SeTl	11	-3.949	-4.293	-1.000e-06	0.00544	0.795	4.288
lieb_000_07853	Dy ₃ EuNa ₄	8	-2.223	-2.331	-1.300e-05	0.00734	1.955	2.924
lieb_000_07907	Ru ₃ Sn ₈ Tb	12	-5.149	-5.352	-6.000e-06	0.00625	0.678	1.516

Table S14. The profile of generated materials with Lieb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
lieb_000_07941	Dy ₅ EuInSn	8	-4.018	-4.18	0.000e+00	0.00524	1.453	1.739
lieb_000_08021	CaDy ₃ Na ₄	8	-2.234	-2.314	0.000e+00	0.00428	1.485	0.707
lieb_000_08028	As ₂ Fe ₄ Rb ₂ Se ₂	10	-5.187	-5.497	4.000e-06	0.00784	0.674	0.837
lieb_000_08053	Ni ₄ Te ₄	8	-4.4	-4.476	-3.000e-06	0.00877	0.435	0.414
lieb_000_08109	Co ₂ Nd ₃ S ₅ Zr ₂	12	-5.422	-6.53	-5.000e-06	0.00768	2.588	3.068
lieb_000_08165	Gd ₃ La ₄ Rh ₄ Sn	12	-6.02	-6.083	-3.000e-05	0.00661	0.248	0.201
lieb_000_08171	Dy ₃ Sn ₉	12	-4.093	-4.324	-3.000e-06	0.00578	1.392	0.909
lieb_000_08271	GeNi ₆ Pd	8	-5.323	-5.408	1.000e-06	0.00502	0.254	0.772
lieb_000_08289	EuGd ₃ Na ₃ Sn	8	-2.396	-2.906	-6.000e-06	0.00961	1.953	1.818
lieb_000_08297	Gd ₃ Sn ₂ SrTl ₂	8	-3.041	-3.903	-2.000e-05	0.00968	2.008	1.42
lieb_000_08298	MnNi ₇	8	-5.765	-5.821	-1.000e-06	0.00552	0.168	0.708
lieb_000_08302	Al ₂ Ni ₆	8	-5.43	-5.467	-1.300e-05	0.00646	0.162	0.138
lieb_000_08313	Al ₂ Co ₄ GaNi	8	-5.569	-5.803	-1.000e-05	0.00871	0.892	1.087
lieb_000_08372	AuCaCeGe ₄ Ru ₃ Tb ₂	12	-5.665	-5.939	-1.000e-06	0.00618	0.423	1.066
lieb_000_08379	As ₃ Cu ₂ Fe ₄ P	10	-5.925	-6.013	-2.000e-06	0.00584	0.31	0.211
lieb_000_08389	CoGd ₃ Mn ₅ Zn ₂	12	-4.143	-5.235	-5.000e-06	0.00582	2.215	2.346
lieb_000_08391	HAsNi ₃ SbUZr	8	-5.755	-6.33	-7.000e-06	0.00729	1.241	1.474
lieb_000_08392	Co ₄ Ga ₂ Mg ₄ P ₂	12	-4.317	-4.601	-1.000e-06	0.0094	1.007	1.495
lieb_000_08414	Sn ₅ Sr ₄ Tb ₃	12	-3.77	-3.859	-1.000e-06	0.00381	0.695	0.692
lieb_000_08444	NaNd ₃ Tl ₄	8	-3.05	-3.254	-2.000e-06	0.00428	0.547	0.44
lieb_000_08459	Al ₄ Ru ₃ Zr	8	-6.395	-6.927	0.000e+00	0.00378	0.434	0.422
lieb_000_08562	CaCdDy ₃ Te ₇	12	-3.731	-4.208	-2.000e-06	0.00349	1.543	2.274
lieb_000_08565	Bi ₂ Rb ₄ Te ₂ Yb ₃	11	-2.827	-2.898	-2.000e-06	0.00493	0.621	0.556
lieb_000_08597	Gd ₃ NaTl ₄	8	-3.035	-3.177	0.000e+00	0.00438	0.403	0.303
lieb_000_08611	Co ₃ GaGeNi ₅ TaZr	12	-6.272	-6.58	2.900e-05	0.00923	0.57	1.717
lieb_000_08656	Cs ₆ Tb ₃	9	-1.457	-1.677	-3.000e-06	0.00279	1.641	3.538
lieb_000_08694	Ni ₈	8	-5.251	-5.412	-6.100e-05	0.00972	0.301	1.931
lieb_000_08740	Ga ₃ GeNi ₃	7	-4.348	-4.477	2.000e-06	0.00543	0.663	0.53
lieb_000_08758	Ba ₄ Ru ₄ Sn ₄	12	-5.216	-5.273	3.000e-06	0.00335	0.154	0.256
lieb_000_08792	CuIrLaMn ₄ PtSiSn ₂	11	-6.193	-6.654	0.000e+00	0.00551	0.649	1.469
lieb_000_08807	Al ₂ GeInLaRu ₃ Si	9	-5.814	-6.044	0.000e+00	0.00881	0.902	0.7
lieb_000_08860	Dy ₃ K ₂ Ni ₃ Te ₄	12	-3.956	-4.378	-1.000e-05	0.00759	1.077	1.898
lieb_000_08912	Gd ₃ Sn ₉	12	-4.042	-4.397	-2.000e-06	0.0074	0.938	2.53
lieb_000_08920	Gd ₃ IrRu ₂ Sn ₅	11	-5.375	-5.845	-4.000e-06	0.00597	1.012	1.43
lieb_000_08941	EuNa ₃ SnYb ₃	8	-1.7	-1.836	2.800e-05	0.00436	1.65	1.348
lieb_000_09002	Bi ₄ CdCs ₄ Yb ₃	12	-2.632	-2.66	0.000e+00	0.00713	0.345	0.481
lieb_000_09014	Ba ₂ Se ₆ Tb ₄	12	-4.92	-5.106	0.000e+00	0.0024	0.487	0.696
lieb_000_09029	Ga ₈ Tb ₃ Zn	12	-3.205	-3.566	0.000e+00	0.00493	0.988	1.107
lieb_000_09067	Dy ₃ La ₂ NdSn ₂	8	-4.818	-4.904	-2.000e-06	0.0065	0.276	0.313
lieb_000_09093	Al ₄ CeGa ₂ Ni ₃ Zn ₂	12	-3.817	-4.124	-7.000e-06	0.00551	0.702	1.775
lieb_000_09100	C ₂ BLa ₂ Ni ₃	8	-6.199	-6.567	-5.000e-06	0.00994	0.744	0.967
lieb_000_09111	H ₈ Co ₃ U	12	-4.361	-4.915	1.000e-06	0.00931	0.869	1.41
lieb_000_09150	CrNi ₅ V	7	-6.326	-6.332	0.000e+00	0.00812	0.099	0.071
lieb_000_09209	AgEuLaNi ₃ SnTl	8	-3.968	-4.34	-1.000e-06	0.00607	0.824	0.844
lieb_000_09247	Fe ₄ Pt ₄	8	-7.002	-7.013	1.000e-05	0.0094	0.086	0.7
lieb_000_09305	AlGd ₄ HgSnY	8	-4.17	-4.418	-1.000e-06	0.00371	1.737	2.062
lieb_000_09315	As ₃ Dy ₃ I ₂ Zn	9	-3.829	-4.361	-1.000e-06	0.00328	0.969	0.882
lieb_000_09317	AlCa ₂ CdINd ₃ Sn ₃ Te	12	-3.38	-3.918	0.000e+00	0.0041	2.176	3.662
lieb_000_09327	AlCo ₇	8	-6.597	-6.616	-2.000e-06	0.00562	0.152	0.708
lieb_000_09335	KSn ₂ SrYb ₄	8	-2.21	-2.319	-1.000e-06	0.00357	0.469	1.325
lieb_000_09355	Nd ₃ Tl ₅	8	-3.207	-3.486	1.400e-05	0.00461	0.509	0.411
lieb_000_09378	Gd ₃ NaPrSn ₂ Sr	8	-3.725	-3.941	-2.000e-06	0.00371	1.453	1.906

Table S14. The profile of generated materials with Lieb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
lieb_000_09388	Ca ₆ Gd ₃ La ₃	12	-3.127	-3.249	-4.000e-06	0.00264	0.826	0.931
lieb_000_09424	Ca ₂ Ga ₄ Mg ₃ Nd ₃	12	-2.888	-3.121	-1.000e-06	0.00431	1.08	0.612
lieb_000_09439	Ba ₂ Br ₂ CaPb ₄ Tb ₃	12	-3.365	-3.678	0.000e+00	0.00354	1.233	0.91
lieb_000_09459	AsNi ₄ P ₅ Rb ₂	12	-4.566	-4.896	-9.000e-06	0.00922	0.924	1.11
lieb_000_09520	Gd ₃ S ₃ Sn ₂ V ₂	10	-5.007	-6.033	2.000e-06	0.00572	1.64	2.337
lieb_000_09572	CoFeNi ₅ Pt	8	-5.672	-5.973	-2.000e-05	0.00705	0.296	1.56
lieb_000_09576	Gd ₅ In ₃	8	-4.113	-4.176	-5.000e-06	0.00424	0.589	0.479
lieb_000_09581	CoGa ₂ Ni ₄ Sb ₂ Zn ₃	12	-3.746	-3.974	0.000e+00	0.00713	0.533	0.546
lieb_000_09591	Al ₆ Mn ₃ Pd ₃	12	-5.442	-5.736	-9.000e-06	0.00486	0.79	0.638
lieb_000_09663	Co ₄ Ge ₄ Y ₄	12	-6.566	-6.659	-3.000e-06	0.00508	0.121	0.156
lieb_000_09666	Al ₅ Ce ₂ Ru ₃	10	-5.907	-6.273	2.000e-06	0.0096	0.624	0.953
lieb_000_09675	Mn ₆ Ni ₆	12	-6.96	-7.164	3.000e-06	0.00965	0.4	0.194
lieb_000_09679	Fe ₃ Pt ₅	8	-6.468	-6.779	-1.000e-06	0.00649	0.518	0.596
lieb_000_09695	Br ₃ Co ₂ Ga ₂ Gd ₃	10	-4.124	-4.441	-2.000e-05	0.00518	1.015	2.137
lieb_000_09737	Fe ₈ Si ₄	12	-7.077	-7.441	-3.800e-05	0.00848	1.451	1.031
lieb_000_09744	Li ₅ Se ₄ Tb ₃	12	-3.843	-3.987	-1.000e-06	0.00565	0.612	1.676
lieb_000_09795	Al ₃ Mn ₃ Pd ₂	8	-6.224	-6.377	0.000e+00	0.00307	0.669	2.769
lieb_000_09797	Nd ₅ Rh ₄ Sn ₃	12	-5.322	-5.983	-3.000e-06	0.00328	0.898	1.602
lieb_000_09805	Dy ₄ Sn ₈	12	-4.359	-4.466	0.000e+00	0.00827	0.858	0.584
lieb_000_09815	Na ₂ Tb ₃ Tl ₃	8	-2.806	-2.911	0.000e+00	0.00492	0.512	0.252
lieb_000_09858	EuNa ₄ Tb ₃	8	-2.264	-2.319	-7.000e-06	0.00532	1.331	2.391
lieb_000_09895	AlEr ₂ Ge ₂ PrRhRu ₃ UZr	12	-6.637	-7.092	-5.000e-06	0.00798	1.003	1.021
lieb_000_09917	Ga ₃ Gd ₅ Sb ₂ Sn ₃	11	-3.887	-4.246	-2.000e-06	0.00741	1.351	1.511
lieb_000_09964	La ₅ Pd ₄ Yb ₃	12	-4.451	-4.655	-4.000e-06	0.00463	0.963	0.564
lieb_000_10104	Eu ₉ Gd ₃	12	-2.426	-2.453	-1.900e-05	0.00292	0.43	0.325
lieb_000_10155	Cs ₃ Tb ₃ Te ₃	9	-3.274	-3.48	4.000e-06	0.00828	1.31	1.924
lieb_000_10239	CeNd ₄ Sn ₂ Sr	8	-4.245	-4.606	-4.000e-06	0.00428	0.825	0.667
lieb_000_10262	Ca ₂ Nd ₃ RuSi ₂ SnSrZn	11	-3.915	-4.386	-2.000e-06	0.00498	2.161	3.381
lieb_000_10324	Cs ₂ Dy ₃ I ₂ PS ₄	12	-4.129	-4.593	0.000e+00	0.00844	0.512	1.77
lieb_000_10336	K ₃ Nd ₃ SnTl	8	-2.395	-2.841	0.000e+00	0.00576	2.872	2.349
lieb_000_10487	Ba ₆ CdPbSbYb ₃	12	-2.045	-2.319	0.000e+00	0.00724	1.261	1.642
lieb_000_10500	Br ₃ Gd ₃ IK	8	-3.008	-3.552	-4.200e-05	0.00914	2.513	3.329
lieb_000_10528	RuSn ₄ Tb ₄	9	-4.617	-5.336	-2.000e-06	0.00763	0.945	1.34
lieb_000_10534	HgI ₈ Nd ₃	12	-3.253	-3.403	-1.000e-06	0.00422	1.109	1.578
lieb_000_10563	BaEuGd ₃ GeNa ₂	8	-2.736	-3.057	-2.400e-05	0.00783	1.261	1.013
lieb_000_10594	AlNiRh ₂ Ru ₃ U	8	-7.898	-8.133	1.000e-06	0.00849	0.959	1.523
lieb_000_10619	Pt ₃ Ru ₄ V	8	-8.028	-8.153	-1.000e-06	0.00859	0.142	0.059
lieb_000_10633	Gd ₃ GeK ₂ MnSnTe ₃	11	-4.021	-4.394	-2.500e-05	0.00455	0.955	1.502
lieb_000_10660	Cl ₃ NaSnTb ₃	8	-3.04	-4.172	-3.000e-06	0.00417	1.695	3.222
lieb_000_10693	Ge ₂ Ru ₄ U ₃ Zn ₃	12	-6.553	-7.121	-4.000e-06	0.00375	1.141	1.621
lieb_000_10695	AuCo ₃ Sb ₄	8	-4.45	-5.016	0.000e+00	0.00612	1.303	1.965
lieb_000_10760	CaNd ₄ Tl ₃	8	-2.998	-3.677	-3.000e-06	0.00588	2.155	3.32
lieb_000_10833	Br ₉ Nd ₃	12	-3.681	-4.283	0.000e+00	0.0053	1.003	1.055
lieb_000_10852	Eu ₄ Ni ₄ P ₄	12	-5.133	-5.2	-1.340e-04	0.00622	0.181	0.194
lieb_000_10897	Al ₆ EuGaPrTb ₃	12	-3.87	-4.091	0.000e+00	0.00291	0.46	0.549
lieb_000_10914	CaGdLiSi ₄ SnTb ₄	12	-4.681	-4.726	-2.000e-06	0.00966	0.227	1.353
lieb_000_10925	MnNi ₄ Si ₃	8	-6.055	-6.297	-5.300e-05	0.00606	0.341	0.893
lieb_000_10950	Co ₁₂	12	-6.786	-6.841	-6.000e-06	0.00544	0.175	0.102
lieb_000_10980	Ca ₂ Gd ₃ Na ₃	8	-2.405	-2.453	-1.000e-06	0.0018	1.355	1.436
lieb_000_11002	AlCuNi ₆	8	-5.214	-5.218	-1.000e-06	0.00827	0.066	0.05
lieb_000_11007	Rb ₂ SbSnYb ₃	7	-1.724	-2.285	-1.000e-06	0.0028	2.069	3.208
lieb_000_11045	I ₄ Se ₄ Tb ₃ Zr	12	-4.831	-5.056	-8.000e-06	0.00357	1.267	2.357

Table S14. The profile of generated materials with Lieb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
lieb_000_11063	KNa ₂ SnSrYb ₃	8	-1.68	-1.745	-7.000e-06	0.00279	0.518	2.014
lieb_000_11101	Gd ₄ IrMg ₂ Rh ₃ Sr ₂	12	-4.745	-4.997	4.000e-06	0.00611	0.943	2.276
lieb_000_11112	Br ₃ Cs ₂ Tb ₃ Te	9	-2.753	-3.5	-1.100e-05	0.00336	1.733	1.549
lieb_000_11153	Bi ₅ Gd ₃	8	-4.544	-4.692	-2.600e-05	0.00823	0.759	0.687
lieb_000_11187	Mn ₃ ScSi ₃ Zn ₅	12	-4.105	-4.572	-1.000e-05	0.00735	0.715	2.295
lieb_000_11199	Co ₄ Fe ₃ Si	8	-7.16	-7.291	7.000e-06	0.00501	0.16	0.174
lieb_000_11224	BaGd ₄ Sn ₂ Te	8	-3.913	-4.483	-1.000e-06	0.00509	1.021	1.786
lieb_000_11245	Gd ₄ I ₄ S ₄	12	-4.966	-4.99	-5.000e-06	0.00581	0.384	0.53
lieb_000_11253	Dy ₄ Rh ₄ Sn ₄	12	-5.756	-5.926	1.000e-06	0.00355	0.506	0.401
lieb_000_11285	BrCdFe ₃ Te ₃	8	-3.958	-4.433	1.000e-06	0.00701	0.598	1.039
lieb_000_11385	PdPt ₄ Ru ₃	8	-6.791	-7.055	-2.000e-06	0.00249	0.45	1.545
lieb_000_11387	Na ₅ Yb ₃	8	-1.268	-1.272	0.000e+00	0.00222	0.111	0.101
lieb_000_11391	Cd ₂ Ga ₄ Ru ₃ SnTh	11	-4.553	-4.894	1.000e-06	0.00384	1.134	1.065
lieb_000_11411	Br ₃ NaTb ₃ Tl	8	-3.06	-3.646	-1.000e-06	0.00878	2.222	2.394
lieb_000_11487	Dy ₃ MgNaPbTl ₂	8	-2.899	-3.306	-1.000e-06	0.00511	0.662	0.28
lieb_000_11558	BaDy ₄ LiSbSn	8	-3.829	-4.077	-1.000e-06	0.0068	1.973	3.343
lieb_000_11574	AgGa ₃ SeTb ₃ Te ₄	12	-3.545	-4.127	-6.000e-06	0.00833	1.771	2.588
lieb_000_11584	Fe ₆ Pt ₂	8	-7.319	-7.521	-2.000e-06	0.0052	0.189	0.182
lieb_000_11609	Dy ₃ Tl ₄ Yb	8	-2.391	-3.353	-1.000e-06	0.00377	2.422	2.918
lieb_000_11640	GaNd ₃ Os ₃ RuSn ₄	12	-5.809	-6.374	-2.000e-06	0.00629	1.07	2.685
lieb_000_11675	Co ₄ Pt ₄	8	-6.396	-6.439	-3.000e-06	0.00821	0.168	0.07
lieb_000_11701	Ga ₂ MgRh ₄ Ru ₃ SrTl	12	-5.345	-5.568	-2.000e-06	0.00445	1.022	0.854
lieb_000_11743	FeMn ₅ OsSi	8	-8.682	-8.74	-1.500e-05	0.00766	0.098	1.386
lieb_000_11754	Mn ₃ Sb ₄	7	-5.237	-6.015	1.000e-06	0.00555	1.249	1.168
lieb_000_11770	BrK ₂ Pt ₂ Sn ₂ Yb ₃	10	-3.006	-3.476	-2.700e-05	0.00948	0.952	3.664
lieb_000_11814	Al ₂ CaGeNi ₂ Ru ₃ Sn	10	-5.371	-5.76	-2.000e-06	0.00678	0.487	0.453
lieb_000_11815	Dy ₃ KTl ₄	8	-2.733	-2.974	0.000e+00	0.00696	0.565	0.509
lieb_000_11871	Ca ₈ Dy ₃ Sb	12	-2.788	-2.823	-1.000e-06	0.00386	0.826	1.134
lieb_000_11881	Ge ₄ LiNi ₃ Sn ₄	12	-4.354	-4.407	-1.000e-06	0.00378	0.794	1.234
lieb_000_11896	Sn ₄ Yb ₈	12	-2.791	-2.864	0.000e+00	0.00474	0.4	0.343
lieb_000_11910	Co ₄ Pt ₄	8	-6.283	-6.437	-1.520e-04	0.00844	0.325	0.352
lieb_000_11959	Gd ₃ Na ₅	8	-2.188	-2.251	-5.100e-05	0.0049	1.321	1.363
lieb_000_11973	BaBr ₇ Gd ₃ Sr	12	-3.524	-3.815	1.000e-06	0.00525	1.491	1.183
lieb_000_11976	AuCl ₄ Gd ₃ LiRb	10	-2.816	-3.914	-1.000e-06	0.00744	2.251	2.976
lieb_000_11989	AsLiNi ₃ Se ₂ Zr	8	-4.966	-5.382	-1.000e-06	0.00744	1.657	1.965
lieb_000_11990	Hg ₄ Yb ₈	12	-1.354	-1.404	0.000e+00	0.00141	0.357	0.286
lieb_000_11992	Al ₂ Ga ₂ NiRu ₃	8	-5.998	-6.186	-1.000e-06	0.00835	0.717	1.675
lieb_000_12031	Ba ₄ Sb ₄ SrTb ₃	12	-3.999	-4.039	-3.000e-06	0.00256	0.464	0.405
lieb_000_12035	Au ₄ GeLa ₂ Tb ₃ Tl ₂	12	-4.026	-4.416	-1.000e-05	0.00894	1.46	1.669
lieb_000_12038	Cs ₄ Ge ₂ Sb ₂ Yb ₄	12	-2.667	-2.699	0.000e+00	0.00153	0.297	0.196
lieb_000_12046	Bi ₄ Co ₃ Eu ₂	9	-4.167	-4.647	0.000e+00	0.00944	0.763	0.883
lieb_000_12061	Co ₅ Fe ₃ Si ₄	12	-6.834	-6.865	-2.000e-06	0.00815	0.108	0.097
lieb_000_12093	Ca ₄ Co ₃ FeP ₄	12	-5.024	-5.696	8.000e-06	0.00773	0.708	2.127
lieb_000_12117	Co ₄ Ga ₅ Ru ₃	12	-5.665	-5.948	-3.000e-06	0.00556	0.831	0.775
lieb_000_12209	Ge ₃ Ni ₆ Y	10	-5.465	-5.639	-2.900e-05	0.00964	0.624	1.181
lieb_000_12230	Co ₃ LiSe ₃ Sm	8	-4.605	-5.158	0.000e+00	0.00813	0.783	1.005
lieb_000_12234	Co ₂ Gd ₅ Sn ₄ V	12	-4.846	-5.399	2.000e-06	0.00582	1.073	2.034
lieb_000_12252	Co ₄ Gd ₄ PrSb ₂ Sn	12	-5.206	-5.65	-1.700e-05	0.00593	0.682	1.439
lieb_000_12258	Ce ₄ Ni ₄ P ₄	12	-6.065	-6.588	-1.000e-06	0.00414	1.289	0.878
lieb_000_12261	CeSn ₂ Tb ₃ Tl ₂	8	-4.859	-4.342	-4.000e-06	0.00764	0.592	2.18
lieb_000_12274	SiTb ₃ Te ₄	8	-4.349	-4.55	-1.000e-06	0.00565	0.761	0.955
lieb_000_12285	Eu ₂ NaTb ₄ Tl	8	-3.076	-3.127	-8.000e-06	0.00767	0.561	2.631

Table S14. The profile of generated materials with Lieb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
lieb_000_12302	As ₂ Na ₄ P ₂ Ru ₄	12	-5.63	-5.681	0.000e+00	0.00373	0.24	0.184
lieb_000_12306	CrGeNi ₆	8	-5.913	-5.927	4.000e-06	0.00979	0.106	0.14
lieb_000_12353	Eu ₅ Gd ₃	8	-2.472	-2.747	-1.000e-06	0.00109	1.165	1.006
lieb_000_12356	LiNi ₅ Si ₂	8	-5.328	-5.445	-2.000e-06	0.00848	0.256	0.168
lieb_000_12357	Gd ₃ PdPt ₃ Sn ₃ Sr ₂	12	-4.938	-5.138	-1.000e-06	0.00819	0.328	1.506
lieb_000_12365	Pd ₂ Tb ₃ Tl ₅	10	-3.275	-3.803	-1.000e-06	0.00729	1.239	0.971
lieb_000_12384	K ₂ LiMg ₃ Nd ₃ SbSn ₂	12	-2.92	-3.108	1.000e-06	0.00798	1.72	2.052
lieb_000_12397	Gd ₃ SbSn ₃	7	-4.415	-4.807	0.000e+00	0.00656	0.877	1.784
lieb_000_12418	Br ₃ EuISeTb ₃	9	-3.159	-4.088	-1.000e-06	0.00511	1.687	3.228
lieb_000_12440	DyLiMn ₃ Se ₂ Zr	8	-5.907	-6.409	4.000e-06	0.00692	0.752	0.903
lieb_000_12457	Gd ₃ Na ₅	8	-2.19	-2.251	1.000e-06	0.00741	1.32	2.322
lieb_000_12462	Cs ₈ PbTb ₃	12	-1.467	-1.7	-1.500e-05	0.00349	1.871	2.603
lieb_000_12486	AlNi ₄ Ti ₂ Zn	8	-5.427	-5.691	1.000e-06	0.00436	1.12	0.988
lieb_000_12535	Ni ₄ Pt ₄	8	-5.629	-5.826	-2.000e-06	0.00519	0.426	0.924
lieb_000_12546	FeNi ₆ Si	8	-5.858	-5.935	-4.000e-06	0.00571	0.138	0.106
lieb_000_12584	Co ₄ Se ₃ Sn	8	-5.375	-5.468	-2.000e-06	0.00583	0.171	0.157
lieb_000_12598	Co ₄ Se ₂ Te ₂	8	-4.737	-5.363	-7.000e-05	0.00819	1.424	0.816
lieb_000_12599	Br ₃ Cs ₂ GaNd ₃ Se ₃	12	-3.859	-4.114	0.000e+00	0.00687	1.027	1.73
lieb_000_12633	Gd ₃ Tl ₅	8	-2.642	-3.334	1.700e-05	0.00355	1.687	1.424
lieb_000_12652	BaCeRh ₃ Sn ₃ Tb ₃	11	-5.296	-5.532	-1.000e-06	0.00711	0.84	0.743
lieb_000_12673	Co ₅ Ga ₂ Pt	8	-5.901	-5.913	8.000e-06	0.00614	0.116	0.741
lieb_000_12677	Tb ₃ Tl ₉	12	-2.746	-2.934	-2.000e-06	0.0045	0.687	0.621
lieb_000_12686	EuGd ₃ KS ₃	8	-3.445	-3.851	-2.000e-06	0.00542	1.482	2.862
lieb_000_12737	BrCl ₄ Gd ₃ Os ₂	10	-4.39	-5.415	-5.000e-06	0.00697	1.953	3.635
lieb_000_12811	CaDy ₃ Ga ₄ GeSr ₃	12	-3.237	-3.34	-2.400e-05	0.00459	0.208	0.425
lieb_000_12866	Br ₅ Tb ₃ V	9	-3.576	-4.291	-1.000e-06	0.00484	1.092	1.764
lieb_000_12902	Dy ₃ SnSr ₄	8	-2.863	-2.945	-5.300e-05	0.00469	1.314	0.76
lieb_000_12904	LiRu ₃ Se ₃ U	8	-6.405	-6.695	0.000e+00	0.00859	0.599	0.615
lieb_000_12950	Br ₄ KTb ₃ TcTe	10	-3.447	-4.397	-3.000e-06	0.00627	1.649	2.326
lieb_000_12991	Co ₃ Mn ₄ Pt	8	-7.704	-7.818	0.000e+00	0.00616	0.157	0.789
lieb_000_12995	As ₅ K ₂ NaNd ₃ Tl	12	-3.89	-4.232	-1.000e-06	0.00589	1.525	1.755
lieb_000_13012	Al ₂ Ca ₃ CdEuTb ₃	10	-2.667	-2.974	-1.000e-06	0.00413	0.429	1.404
lieb_000_13046	Dy ₃ Eu ₂ LaNaSn	8	-3.411	-3.468	-5.000e-06	0.00548	1.2	1.438
lieb_000_13057	AuCoGaRu ₅ SiV ₃	12	-7.344	-7.749	-2.000e-06	0.00538	0.833	1.314
lieb_000_13083	Co ₃ Ni ₇ Ti ₂	12	-6.257	-6.403	-1.800e-05	0.00953	0.197	0.317
lieb_000_13092	GeNa ₄ Ru ₃	8	-3.295	-4.199	1.000e-06	0.00674	1.713	2.372
lieb_000_13095	Eu ₄ Yb ₄	8	-1.647	-1.655	-3.000e-06	0.00092	0.191	0.141
lieb_000_13119	Co ₃ GaLa ₈	12	-5.129	-5.401	9.000e-06	0.00748	0.699	0.798
lieb_000_13153	Ni ₈	8	-5.351	-5.413	-1.600e-05	0.00522	0.167	0.099
lieb_000_13186	EuGa ₃ SnTb ₃	8	-3.956	-4.082	-4.000e-06	0.00613	0.306	0.432
lieb_000_13188	BrCaNd ₃ Sn ₃	8	-3.59	-4.34	-3.000e-05	0.00629	1.043	1.159
lieb_000_13191	BiCdRb ₂ SbSn ₂ SrTb ₃	11	-3.313	-3.44	-2.000e-06	0.00554	0.548	0.749
lieb_000_13193	Al ₂ Fe ₃ Ni ₆ V	12	-5.977	-6.351	-1.000e-06	0.00594	0.55	0.335
lieb_000_13219	LiPt ₄ Ru ₃	8	-6.737	-6.754	0.000e+00	0.00423	0.109	1.393
lieb_000_13234	AlDy ₃ I ₅ Sb	10	-2.589	-3.617	-1.400e-05	0.00618	1.897	2.738
lieb_000_13273	Co ₅ Ga ₃	8	-5.502	-5.601	-1.000e-05	0.00508	0.776	1.252
lieb_000_13302	Ga ₄ Gd ₇ Ge	12	-4.127	-4.435	-6.000e-06	0.00522	0.903	2.741
lieb_000_13330	Ge ₂ Ni ₃ Sn ₄	9	-4.351	-4.591	1.000e-06	0.00664	1.183	2.307
lieb_000_13340	AlGaMn ₅ Ni	8	-6.93	-7.113	-1.400e-05	0.00481	0.185	0.235
lieb_000_13351	Br ₈ Dy ₄	12	-3.797	-4.128	0.000e+00	0.0033	0.994	0.82
lieb_000_13353	Co ₅ GeMnNi ₅	12	-5.803	-6.261	-9.000e-06	0.00579	0.86	0.43
lieb_000_13423	BGe ₃ Ru ₄ Se	9	-6.174	-6.738	-1.000e-06	0.00671	0.81	0.589

Table S14. The profile of generated materials with Lieb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
lieb_000_13462	Ga ₄ Ni ₄	8	-4.365	-4.411	-3.300e-05	0.00888	0.279	0.15
lieb_000_13488	Fe ₅ Ni ₅ U ₂	12	-7.383	-7.522	-1.000e-06	0.00634	0.295	0.311
lieb_000_13539	Al ₃ Ni ₇ Ti ₂	12	-5.785	-5.931	-8.000e-06	0.00974	0.228	0.332
lieb_000_13615	Al ₂ BaGeKSr ₂ Tl ₂ Yb ₃	12	-2.189	-2.397	0.000e+00	0.00205	1.077	2.261
lieb_000_13627	CaK ₄ Nd ₃ Sb ₄	12	-3.633	-3.729	2.000e-06	0.00569	1.001	0.802
lieb_000_13672	Gd ₈ Sb ₄	12	-4.898	-5.024	1.000e-06	0.00489	0.576	0.344
lieb_000_13691	Co ₇ Fe	8	-6.931	-6.994	1.000e-06	0.00581	0.124	0.102
lieb_000_13695	AsAuGaI ₂ IrSmTb ₃ Te	11	-4.111	-4.651	-2.000e-06	0.00436	2.943	1.773
lieb_000_13711	GaGd ₃ I ₄	8	-3.09	-3.615	0.000e+00	0.00436	1.365	2.939
lieb_000_13712	BaEuNa ₂ Nd ₄	8	-2.867	-2.956	-9.000e-06	0.00429	1.711	2.644
lieb_000_13750	Dy ₃ Na ₅	8	-2.13	-2.215	0.000e+00	0.00464	1.35	0.86
lieb_000_13752	Ba ₂ Se ₅ SnSrYb ₃	12	-3.506	-4.127	-1.000e-06	0.00368	1.408	1.807
lieb_000_13804	Fe ₃ Ga ₆ Ni ₃	12	-4.776	-4.965	3.000e-06	0.00642	0.897	0.704
lieb_000_13866	Cl ₂ LiMn ₅ O ₄	12	-6.116	-6.63	0.000e+00	0.00602	0.728	1.38
lieb_000_13877	BiCaGd ₃ Sn ₇	12	-3.943	-4.247	-2.000e-06	0.00797	0.644	0.666
lieb_000_13933	CaDy ₃ Gd ₂ Se ₅ Sr	12	-4.321	-4.932	-1.000e-06	0.00585	1.525	2.555
lieb_000_13947	BrGd ₄ I ₃	8	-3.327	-3.846	0.000e+00	0.00372	1.181	1.848
lieb_000_13973	Al ₄ LiMn ₂ NiRu ₃ Ta	12	-6.372	-6.873	-3.000e-06	0.00801	0.851	1.583
lieb_000_14061	Ca ₃ Gd ₃ NaSn	8	-3.089	-3.152	-1.900e-05	0.00489	0.358	2.213
lieb_000_14080	Ca ₇ CdDy ₃ Ga	12	-2.512	-2.583	-2.000e-06	0.00385	0.696	0.662
lieb_000_14153	BaCaGd ₄ LaMgTl ₄	12	-3.158	-3.287	0.000e+00	0.00368	0.612	0.955
lieb_000_14186	CoGa ₄ LiRu ₃ TiUZr	12	-6.349	-6.593	-5.000e-06	0.00645	0.488	0.52
lieb_000_14197	FeNi ₇	8	-5.692	-5.701	-4.000e-06	0.00704	0.071	0.071
lieb_000_14218	CaCeGd ₃ Sr ₃	8	-3.007	-3.031	-3.500e-05	0.00304	0.334	1.048
lieb_000_14228	AlCrFe ₄ NbPt	8	-7.614	-7.839	-1.600e-05	0.0061	0.669	1.789
lieb_000_14246	Ce ₇ Nd ₃ PbSc	12	-5.091	-5.474	-3.400e-05	0.00726	0.873	0.706
lieb_000_14323	Fe ₂ Ni ₈ TiU	12	-6.651	-6.719	-8.000e-06	0.00558	0.124	0.165
lieb_000_14332	H ₄ LaMn ₃ Ni	9	-4.405	-5.571	0.000e+00	0.00552	1.415	2.078
lieb_000_14336	Cl ₈ Gd ₄	12	-3.757	-4.687	-1.000e-05	0.00281	1.459	1.12
lieb_000_14340	GaMn ₃ Pd ₂ Pt ₂	8	-6.484	-6.553	-4.000e-06	0.00583	0.312	1.578
lieb_000_14354	Tl ₃ Yb ₅	8	-1.838	-2.099	3.000e-06	0.00269	1.18	1.332
lieb_000_14380	AuCdSn ₄ Yb ₅	11	-2.468	-3.013	-5.000e-06	0.00473	2.115	3.499
lieb_000_14407	AlDy ₃ Eu ₂ Tl ₂	8	-3.308	-3.406	-1.000e-06	0.00444	0.534	1.341
lieb_000_14428	BiCdEuNd ₄ Sn	8	-3.8	-4.063	1.000e-06	0.00862	0.628	1.301
lieb_000_14510	Dy ₃ Se ₄ Tl	8	-4.474	-5.214	-4.000e-06	0.00607	2.022	2.027
lieb_000_14561	Ca ₂ Cd ₂ Eu ₂ Mg ₃ Nd ₃	12	-2.305	-2.389	2.000e-06	0.00839	0.492	0.603
lieb_000_14600	As ₃ CoFe ₆ Ni	11	-6.381	-6.666	-7.000e-06	0.00833	0.592	1.058
lieb_000_14611	Cs ₅ Tb ₃	8	-1.563	-1.787	-4.000e-06	0.00294	0.973	1.218
lieb_000_14626	Cl ₆ Tb ₃	9	-4.38	-4.585	-1.400e-05	0.00773	0.645	0.557
lieb_000_14660	Eu ₂ Gd ₃ In ₂ Tl	8	-3.2	-3.405	1.000e-06	0.00738	0.458	0.423
lieb_000_14664	Ga ₇ Nd ₄ Sn	12	-3.694	-4.259	2.000e-06	0.00811	1.378	2.373
lieb_000_14673	ErIn ₇ Ru ₃ Yb	12	-4.306	-4.409	4.000e-06	0.0081	0.551	0.579
lieb_000_14674	BaDy ₃ GaLaSn ₂	8	-3.998	-4.182	-1.000e-06	0.00321	0.52	0.608
lieb_000_14676	Pt ₅ Ru ₃	8	-6.584	-7.226	1.000e-06	0.00389	0.437	0.363
lieb_000_14722	H ₂ CuNa ₂ Ni ₃ S ₄	12	-3.755	-4.199	2.000e-06	0.00947	0.652	1.128
lieb_000_14744	Mg ₄ Nd ₃ Te ₅	12	-3.182	-3.743	1.000e-06	0.00472	1.406	2.4
lieb_000_14749	EuNa ₄ Nd ₃	8	-2.378	-2.415	-1.100e-05	0.00371	1.339	1.558
lieb_000_14751	Ba ₂ Nd ₄ Sn ₂	8	-3.667	-4.073	-8.000e-06	0.00402	2.031	1.649
lieb_000_14780	Fe ₃ Ga ₇ NiTi	12	-4.742	-4.961	4.000e-06	0.00892	0.714	0.795
lieb_000_14806	AgCaK ₃ SbYb ₃	9	-1.586	-1.906	0.000e+00	0.00399	2.636	1.878
lieb_000_14854	Dy ₃ GdITe ₇	12	-3.904	-4.584	-4.500e-05	0.00875	1.16	3.357
lieb_000_14887	AlCo ₃ Ge ₄ NiPrSnY	12	-5.436	-5.611	1.000e-06	0.00634	0.594	0.633

Table S14. The profile of generated materials with Lieb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
lieb_000_14891	Co ₇ Fe	8	-6.925	-6.994	0.000e+00	0.00523	0.119	0.12
lieb_000_14910	Br ₄ FeMn ₃	8	-4.697	-4.987	-1.000e-06	0.00529	0.611	0.56
lieb_000_14928	Na ₄ Nd ₄	8	-2.698	-2.735	-1.000e-06	0.00292	1.2	1.331
lieb_000_14935	LuSn ₂ Tb ₅	8	-4.686	-4.791	-1.000e-06	0.00536	0.291	0.205
lieb_000_14944	Au ₂ Mn ₄ Na ₂ S ₄	12	-5.264	-5.432	5.000e-06	0.00702	0.233	0.717
lieb_000_14948	AlGe ₃ Ni ₃ Ta	8	-5.726	-5.775	-8.000e-06	0.00997	0.283	0.19
lieb_000_14977	Ni ₁₀ TiV	12	-5.958	-6.132	5.000e-06	0.00766	0.242	0.435
lieb_000_15002	Gd ₃ Sb ₂ Sn ₂ Sr	8	-3.773	-4.617	0.000e+00	0.00441	1.465	2.11
lieb_000_15036	Gd ₅ Sr ₃ Tl ₄	12	-3.004	-3.227	-7.000e-06	0.0031	0.819	0.786
lieb_000_15040	CoCu ₂ Mn ₃ Se ₄	10	-5.494	-5.525	-3.000e-06	0.00653	0.11	0.1
lieb_000_15064	Nd ₇ Tl	8	-4.351	-4.462	-2.000e-06	0.00197	0.363	0.372
lieb_000_15115	AlFe ₇ Rh ₃ Ti	12	-7.435	-7.62	3.000e-06	0.00487	0.318	0.267
lieb_000_15193	Ag ₃ Cl ₅ Gd ₃ Sn	12	-3.173	-3.949	-2.000e-06	0.00824	1.083	2.071
lieb_000_15198	Gd ₃ NaSnTl ₃	8	-3.158	-3.439	-5.000e-06	0.00467	0.704	1.442
lieb_000_15199	Cr ₃ Gd ₃ Se ₅ Ti	12	-5.622	-6.258	0.000e+00	0.00748	0.707	1.964
lieb_000_15222	As ₄ CaNd ₅ Te ₂	12	-4.927	-5.705	0.000e+00	0.00389	2.323	3.309
lieb_000_15231	Cs ₈ Nd ₃ Sn	12	-1.626	-1.956	1.000e-06	0.00238	2.515	3.308
lieb_000_15245	FePtRh ₂ Ru ₄	8	-7.917	-8.121	-1.000e-06	0.0064	0.235	0.203
lieb_000_15252	K ₄ LiNd ₃ Sn ₃	11	-3.01	-3.07	1.000e-06	0.00387	0.126	0.237
lieb_000_15262	P ₂ Ru ₃ Se ₅ Sr	11	-5.314	-5.712	-9.000e-06	0.00886	0.816	0.942
lieb_000_15274	GaNi ₆ Sn	8	-5.02	-5.061	-2.000e-06	0.00764	0.343	0.459
lieb_000_15280	Mn ₃ Pt ₅	8	-7.099	-7.149	-8.000e-06	0.00441	0.118	0.139
lieb_000_15303	Fe ₄ GaGe ₂ PuRh ₂	10	-6.76	-7.31	-3.000e-06	0.00343	1.071	2.471
lieb_000_15305	Na ₂ Tl ₃ Yb ₃	8	-1.697	-1.907	-1.000e-06	0.0042	1.208	0.526
lieb_000_15361	CuNi ₃ S ₂ Se ₂	8	-4.614	-4.672	-2.000e-06	0.00631	0.137	0.833
lieb_000_15375	Co ₃ Ni ₈	11	-5.535	-5.648	1.000e-06	0.00474	0.273	0.26
lieb_000_15395	Co ₃ LaPrSb ₃	8	-5.178	-5.747	7.000e-06	0.00988	0.532	0.569
lieb_000_15423	AlGd ₅ SbSn	8	-4.395	-4.75	0.000e+00	0.00998	1.668	1.523
lieb_000_15447	BrCaGd ₃ Ge ₂ ISb ₄	12	-3.927	-4.39	-3.000e-06	0.00516	1.468	2.269
lieb_000_15456	Ba ₂ CaGd ₄ PbSe ₃	11	-3.854	-4.4	0.000e+00	0.00543	1.244	1.309
lieb_000_15479	BaBiTb ₃ Te ₆ Tl	12	-4.178	-4.392	-2.000e-06	0.0055	1.117	1.24
lieb_000_15484	Co ₂ Fe ₃ Pt ₃	8	-6.836	-6.993	-1.000e-05	0.00546	0.271	1.065
lieb_000_15544	AsBrEuKSbTb ₃	8	-3.18	-4.077	-9.000e-06	0.00748	1.869	2.396
lieb_000_15563	Gd ₃ I ₈ Tl	12	-3.387	-3.48	0.000e+00	0.00532	0.387	0.606
lieb_000_15663	AlNi ₄ PtZn ₂	8	-4.353	-4.53	-5.000e-06	0.00458	0.335	0.306
lieb_000_15667	Ce ₃ NaTb ₄	8	-4.287	-4.466	-8.000e-06	0.00332	0.451	0.347
lieb_000_15686	CdDy ₃ Ga ₄ Ti ₄	12	-4.572	-4.98	1.000e-06	0.00263	0.622	1.061
lieb_000_15690	Bi ₃ Gd ₄ GeP ₃ Rh	12	-5.055	-5.482	1.000e-06	0.00546	1.487	2.031
lieb_000_15724	Ni ₈	8	-5.382	-5.411	0.000e+00	0.0043	0.122	0.147
lieb_000_15748	Fe ₄ Ni ₇ V	12	-6.339	-6.623	-3.500e-05	0.00812	0.437	0.625
lieb_000_15763	Co ₈	8	-6.795	-6.841	-4.000e-06	0.00641	0.194	0.13
lieb_000_15825	S ₆ Tb ₃ Tl ₂	11	-4.982	-5.208	0.000e+00	0.00262	0.809	1.513
lieb_000_15828	AlCoDy ₆ GaV ₂	11	-4.811	-5.43	-7.000e-06	0.00383	1.304	1.539
lieb_000_15837	AlAsCaSnSrTb ₃	8	-3.742	-4.191	-2.100e-05	0.00524	1.541	5.162
lieb_000_15850	CeDy ₃ EuGeSnTl	8	-4.462	-4.338	-8.000e-06	0.00437	0.623	1.332
lieb_000_15869	Al ₂ Dy ₃ Se ₇	12	-4.799	-5.028	-9.000e-06	0.00576	0.772	1.251
lieb_000_15889	GaNi ₁₀	11	-5.086	-5.189	6.000e-06	0.00905	0.351	0.496
lieb_000_15916	Cs ₄ RbYb ₃	8	-0.609	-0.92	4.000e-07	0.00285	3.277	6.095
lieb_000_15932	Co ₅ Pt ₃	8	-6.478	-6.557	0.000e+00	0.00808	0.218	0.194
lieb_000_15986	CoFe ₃ NiRhSi ₂	8	-7.009	-7.087	-2.000e-06	0.00461	0.349	2.062
lieb_000_15997	CaGe ₅ Nd ₄ Pd ₂	12	-4.69	-5.074	-2.000e-06	0.00892	0.923	1.588
lieb_000_16024	Ga ₈ Ru ₃ U	12	-5.084	-5.326	0.000e+00	0.00717	0.484	0.615

Table S14. The profile of generated materials with Lieb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
lieb_000_16035	AlBa ₂ Ga ₄ GeNd ₃ Sn	12	-3.569	-3.85	0.000e+00	0.00579	1.012	2.746
lieb_000_16058	Pt ₃ Ru ₃ U ₂	8	-8.865	-9.12	3.000e-06	0.00388	0.24	0.135
lieb_000_16120	Br ₄ GeS ₄ Tb ₃	12	-4.645	-4.864	-1.000e-06	0.00952	0.749	2.936
lieb_000_16144	Cs ₂ Dy ₃ S ₂ TaTe ₄	12	-5.131	-5.185	1.000e-06	0.00314	0.351	0.457
lieb_000_16207	Gd ₆ ISiSn ₄	12	-4.038	-4.792	1.000e-06	0.00741	1.298	2.705
lieb_000_16215	AlCo ₃ Ni ₄	8	-5.713	-5.897	-3.000e-06	0.0032	0.304	0.171
lieb_000_16232	Fe ₃ Ga ₅ Li ₂ U ₂	12	-5.106	-5.577	-1.000e-06	0.00387	0.573	0.959
lieb_000_16251	Fe ₆ MnNi	8	-7.712	-7.83	-1.300e-05	0.00315	0.196	0.147
lieb_000_16265	HgSbSn ₂ Yb ₈	12	-2.393	-2.516	1.000e-06	0.00441	0.395	0.785
lieb_000_16271	Dy ₃ Hg ₄ Te ₅	12	-2.155	-3.087	-3.000e-06	0.00775	2.614	2.292
lieb_000_16304	Co ₃ Ni ₅	8	-5.839	-5.901	1.000e-05	0.00559	0.127	0.104
lieb_000_16350	Co ₂ Mn ₄ N ₂ Ti ₂	10	-7.697	-8.411	-3.400e-05	0.00993	0.717	1.046
lieb_000_16391	Dy ₃ KNa ₂ Sb ₂	8	-2.82	-3.461	1.000e-06	0.00375	2.065	3.163
lieb_000_16393	Ni ₄ Pt ₃ Ti	8	-6.343	-6.347	-4.000e-06	0.00782	0.059	0.714
lieb_000_16425	Fe ₅ MnNi ₂	8	-7.368	-7.466	-7.000e-06	0.00823	0.162	0.127
lieb_000_16457	As ₆ Co ₃ KNa ₂	12	-4.44	-4.589	-3.000e-06	0.00912	0.259	0.799
lieb_000_16485	Ni ₁₂	12	-5.237	-5.418	-1.900e-05	0.00698	0.357	0.266
lieb_000_16528	CeGaMn ₃ NdP ₆	12	-6.3	-6.562	-1.200e-05	0.0071	0.505	1.95
lieb_000_16541	Ce ₄ Mn ₄ Pt ₄	12	-7.032	-7.306	0.000e+00	0.0075	0.686	0.743
lieb_000_16581	Dy ₃ Pd ₉	12	-4.93	-5.761	-1.000e-06	0.00213	0.898	1.056
lieb_000_16585	AlNi ₇	8	-5.31	-5.451	-1.300e-05	0.00477	0.238	0.834
lieb_000_16625	Co ₃ Ga ₃ GdGeNiRu ₂	11	-5.7	-5.764	-1.000e-06	0.00595	0.138	1.721
lieb_000_16629	KNa ₃ TlYb ₃	8	-1.366	-1.388	-2.000e-06	0.00399	0.437	0.224
lieb_000_16686	Fe ₄ Ga ₇ Ge	12	-4.693	-4.895	-1.000e-06	0.00477	0.206	0.432
lieb_000_16696	Co ₂ Ni ₉ Ti	12	-5.914	-5.984	-5.000e-06	0.0065	0.26	0.187
lieb_000_16707	BrKSn ₂ SrTb ₃	8	-2.895	-3.643	0.000e+00	0.00258	1.918	2.148
lieb_000_16725	BaEuNd ₃ SnSrTl	8	-2.872	-3.397	0.000e+00	0.00446	2.024	1.541
lieb_000_16755	Cs ₅ Yb ₃	8	-0.697	-0.9	-1.480e-05	0.00311	1.432	5.982
lieb_000_16824	CsI ₄ Tl ₃ Yb ₃	11	-2.026	-2.373	-5.000e-06	0.003	1.789	3.0
lieb_000_16853	Ba ₄ Gd ₃ LiSn ₄	12	-3.762	-3.8	-1.000e-06	0.00336	0.348	0.302
lieb_000_16892	Co ₇ Fe	8	-6.927	-6.994	-7.000e-06	0.00665	0.137	0.099
lieb_000_16912	AlGa ₂ Ru ₃ Y ₂	8	-6.06	-6.564	-7.000e-06	0.00502	0.887	0.95
lieb_000_16919	CdI ₇ Tb ₃ Te	12	-3.148	-3.563	0.000e+00	0.00602	0.747	1.12
lieb_000_16925	BiISbSnTb ₃ Tl	8	-3.533	-4.24	-1.300e-05	0.00779	2.193	2.79
lieb_000_16926	AgBr ₂ CdCsNd ₃ P ₄	12	-3.621	-4.448	0.000e+00	0.00619	1.717	3.052
lieb_000_16940	CdCe ₃ Fe ₄ GdTb ₃	12	-5.412	-5.864	7.000e-06	0.00628	1.788	1.396
lieb_000_16949	Mn ₄ S ₂ Se ₂	8	-6.478	-6.634	-4.000e-06	0.00749	0.346	0.194
lieb_000_16956	H ₅ CdFe ₃ Y ₃	12	-4.549	-5.235	-6.500e-05	0.0087	0.901	1.186
lieb_000_16965	Dy ₃ EuRh ₄ Sn ₄	12	-5.29	-5.6	-3.000e-06	0.00627	0.989	1.144
lieb_000_16969	Br ₅ Tb ₃ V	9	-3.643	-4.311	-1.200e-05	0.00574	1.867	2.679
lieb_000_16996	Ni ₁₂	12	-5.215	-5.417	2.000e-06	0.00756	0.448	0.218
lieb_000_17013	Dy ₃ EuNaSn ₂ Yb	8	-3.254	-3.571	-2.000e-06	0.00339	1.407	1.784
lieb_000_17018	LaNd ₅ Te ₆	12	-4.508	-5.241	0.000e+00	0.00405	1.636	3.899
lieb_000_17038	Ga ₃ Ru ₄ U	8	-7.13	-7.302	-5.000e-06	0.00471	0.807	0.843
lieb_000_17069	CaCo ₄ Gd ₇	12	-4.951	-5.235	1.000e-05	0.00659	1.052	1.358
lieb_000_17080	CeEuMo ₂ Sn ₂ Yb ₆	12	-3.514	-3.871	1.000e-06	0.0061	1.132	1.084
lieb_000_17083	BaI ₃ PbTb ₃ Te ₃	11	-3.653	-4.141	-6.000e-06	0.00623	1.212	2.659
lieb_000_17094	CaFe ₂ Ga ₃ Nd ₄ SbSn	12	-4.425	-4.784	-1.000e-06	0.00516	0.906	0.803
lieb_000_17134	Al ₅ Fe ₄ Ti ₃	12	-6.087	-6.539	-1.000e-06	0.00378	1.197	1.75
lieb_000_17154	Pd ₉ Ru ₃	12	-5.779	-6.093	-4.000e-06	0.00442	0.541	0.439
lieb_000_17193	AlGeMn ₃ NiY ₂ Zn	9	-5.795	-6.211	-3.000e-06	0.00552	0.574	0.655
lieb_000_17196	EuFeIn ₂ Tb ₄	8	-4.062	-4.272	-3.000e-06	0.00902	1.041	1.573

Table S14. The profile of generated materials with Lieb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
lieb_000_17210	Ba ₂ Dy ₃ Eu ₂ P ₄ Sn	12	-4.421	-4.783	1.000e-06	0.00686	1.363	1.226
lieb_000_17229	Co ₄ Se ₄	8	-5.426	-5.49	0.000e+00	0.00619	0.119	0.708
lieb_000_17279	CaEuKSb ₂ Yb ₃	8	-2.359	-2.687	-3.000e-06	0.00345	1.626	2.649
lieb_000_17321	Dy ₃ Sn ₂ Te ₇	12	-4.03	-4.379	-5.000e-06	0.00806	1.116	1.142
lieb_000_17410	Eu ₅ Gd ₃	8	-2.263	-2.761	0.000e+00	0.00217	1.947	1.085
lieb_000_17431	Ba ₂ LaPd ₂ SbSrYb ₃	10	-3.11	-3.414	-8.000e-06	0.00467	1.619	3.822
lieb_000_17438	AlMn ₃ Pt ₂ Zn ₂	8	-5.597	-5.765	-1.000e-06	0.00699	0.296	1.529
lieb_000_17460	NaSr ₂ Tl ₂ Yb ₃	8	-1.353	-1.849	-3.000e-06	0.00495	1.805	1.314
lieb_000_17551	GeLi ₃ Mn ₃ PtSi ₂ Ta ₂	12	-6.419	-6.637	1.000e-06	0.00391	0.537	0.709
lieb_000_17612	SnTb ₃ Tl ₄	8	-3.487	-3.664	3.000e-06	0.00382	0.302	1.289
lieb_000_17617	Rh ₄ Se ₃ Tb ₅	12	-5.664	-6.03	-2.800e-05	0.00489	0.727	0.517
lieb_000_17664	Ga ₄ Mn ₃ NSn ₄	12	-4.363	-5.075	-2.000e-06	0.00771	0.655	0.692
lieb_000_17706	Fe ₃ GaNi ₄	8	-5.818	-6.08	1.000e-06	0.0083	0.301	0.169
lieb_000_17741	Co ₃ O ₄ Rb ₂	9	-5.328	-5.664	-7.000e-06	0.0081	0.656	0.806
lieb_000_17746	Br ₈ SiTb ₃	12	-3.758	-4.066	-4.000e-06	0.00551	0.431	1.03
lieb_000_17755	As ₂ BrGd ₃ Na ₂ STe ₂	11	-4.221	-4.615	0.000e+00	0.00805	0.887	1.554
lieb_000_17789	AlNi ₉ Ti	11	-5.486	-5.707	0.000e+00	0.00891	0.619	1.054
lieb_000_17790	Li ₅ NiPRu ₄ Sn	12	-4.86	-5.146	-2.600e-05	0.00652	0.486	1.856
lieb_000_17804	GeLi ₂ Mn ₆ Si ₃	12	-6.131	-6.453	-1.000e-06	0.00518	0.74	0.758
lieb_000_17817	Fe ₄ Ni ₈	12	-6.063	-6.251	0.000e+00	0.00713	0.378	0.406
lieb_000_17822	Dy ₂ PdRu ₃ TiZn	8	-6.275	-6.599	-1.000e-06	0.00883	0.989	3.504
lieb_000_17838	Cs ₄ P ₄ Yb ₄	12	-3.285	-3.382	-1.000e-06	0.00243	0.538	0.339
lieb_000_17845	Ni ₇ V	8	-5.931	-5.989	-1.500e-05	0.00464	0.161	0.163
lieb_000_17863	Gd ₄ Ru ₄ Sn ₃ Sr	12	-5.676	-5.895	-9.000e-06	0.00627	0.562	0.606
lieb_000_17866	In ₅ Tb ₃	8	-3.725	-3.735	2.000e-06	0.00304	0.594	0.55
lieb_000_17922	Na ₄ Se ₅ Tb ₃	12	-3.822	-4.275	-3.000e-06	0.00296	1.338	2.501
lieb_000_17933	Co ₃ SnSrTe ₂ Tl	8	-3.886	-4.465	0.000e+00	0.00619	0.763	1.708
lieb_000_17992	As ₄ CdGd ₃ K ₄	12	-3.73	-3.785	0.000e+00	0.00329	0.287	0.388
lieb_000_17999	S ₈ Tb ₄	12	-5.571	-5.863	0.000e+00	0.00574	1.415	2.284
lieb_000_18020	ISe ₄ Tb ₃	8	-4.831	-5.307	-3.000e-06	0.0037	1.568	1.453
lieb_000_18056	Ni ₁₁ Ti	12	-5.726	-5.788	-3.000e-06	0.00775	0.246	0.197
lieb_000_18099	Al ₄ Fe ₃ Ti ₅	12	-6.596	-6.863	-2.000e-06	0.00572	0.939	0.839
lieb_000_18134	CdGe ₄ Nd ₄ TlZn	11	-3.744	-4.239	-8.300e-05	0.0096	1.214	1.957
lieb_000_18148	Au ₃ GaNaTl ₄ Yb ₃	12	-2.419	-2.661	-1.000e-06	0.00387	1.73	1.36
lieb_000_18157	LaNaSn ₃ Tb ₃	8	-3.825	-4.334	-2.000e-06	0.00875	1.948	1.889
lieb_000_18160	Dy ₃ LaNa ₂ PbSb	8	-3.096	-3.891	-1.000e-06	0.00936	2.395	1.945
lieb_000_18182	Co ₈	8	-6.78	-6.842	-5.000e-06	0.00829	0.134	0.692
lieb_000_18195	Na ₅ Yb ₃	8	-1.265	-1.273	2.200e-05	0.00093	0.269	1.106
lieb_000_18205	Dy ₂ Ni ₅	7	-5.273	-5.39	-1.000e-06	0.00923	0.331	0.529
lieb_000_18247	Al ₂ Fe ₈ UV	12	-7.578	-7.828	-6.000e-05	0.00659	0.399	0.41
lieb_000_18301	Bi ₂ Pd ₆ Tb ₄	12	-5.175	-5.485	1.000e-06	0.00574	0.691	0.895
lieb_000_18331	GeNi ₁₃ Sn ₄	8	-4.218	-4.512	-1.000e-06	0.0081	1.256	3.346
lieb_000_18332	Na ₃ Sn ₂ Yb ₃	8	-2.014	-2.268	0.000e+00	0.00282	0.646	0.985
lieb_000_18359	Ag ₂ Br ₅ SnTb ₃ Zn	12	-3.05	-3.422	-2.000e-06	0.004	1.452	2.453
lieb_000_18368	Al ₂ AsLaSn ₂ Tb ₃	9	-4.288	-4.734	-1.000e-06	0.00541	0.799	2.419
lieb_000_18375	Br ₅ Gd ₃ Se	9	-3.204	-4.439	-2.000e-06	0.0024	2.08	3.641
lieb_000_18376	Co ₃ CuNd ₃ Sb	8	-5.123	-5.619	1.600e-05	0.00936	1.306	2.741
lieb_000_18378	CuRu ₃ S ₄	8	-6.161	-6.197	-4.000e-06	0.00855	0.169	0.197
lieb_000_18427	Na ₂ SbSnSrTb ₃	8	-2.868	-3.552	-2.000e-06	0.00575	2.302	2.209
lieb_000_18456	Co ₆ Mn ₂	8	-7.253	-7.4	1.000e-06	0.00648	0.164	0.19
lieb_000_18459	Fe ₄ MnSiU ₂	8	-8.702	-8.817	1.000e-06	0.00977	0.397	0.626
lieb_000_18461	Cs ₆ Nd ₃	9	-1.593	-1.765	6.000e-06	0.00317	1.704	1.946

Table S14. The profile of generated materials with Lieb lattice structures after DFT relaxation (continued)

Material ID	Formula	N	E _{start}	E _{final}	E _{conv}	F _{max}	d _{latt}	d _{xy}
lieb_000_18465	La ₂ Ni ₅ Ru ₃	10	-6.19	-6.514	-1.000e-06	0.00818	0.566	0.395
lieb_000_18504	AsBrI ₂ Tb ₃	7	-3.933	-4.344	-3.000e-06	0.00176	1.521	1.11
lieb_000_18530	Pt ₅ Ru ₃	8	-7.075	-7.211	3.000e-06	0.00451	0.159	0.07
lieb_000_18554	Dy ₄ EuInNd	7	-3.71	-3.892	-2.000e-06	0.00407	0.78	3.685
lieb_000_18561	GaGd ₃ I ₈	12	-3.344	-3.465	-1.000e-06	0.00321	0.519	0.348
lieb_000_18634	Mn ₃ Pt ₄ V	8	-7.552	-7.641	-9.000e-06	0.00623	0.243	0.256
lieb_000_18638	Co ₈	8	-6.79	-6.842	-6.000e-06	0.00676	0.117	0.088
lieb_000_18641	Mn ₃ Se ₇ Sr ₂	12	-4.724	-5.188	0.000e+00	0.00678	0.706	1.663
lieb_000_18648	BiDy ₃ EuInSnSr	8	-3.621	-3.799	-2.000e-06	0.00503	1.386	1.432
lieb_000_18667	Bi ₂ Dy ₃ LuTl ₂	8	-3.971	-4.098	-1.000e-06	0.0086	0.36	0.273
lieb_000_18683	Fe ₄ Se ₄	8	-6.083	-6.149	-1.000e-06	0.00685	0.218	0.255
lieb_000_18685	Bi ₂ EuNaRbYb ₃ Zn	9	-1.899	-2.242	1.000e-06	0.00746	1.034	4.334
lieb_000_18690	Dy ₄ InTl ₃	8	-3.678	-3.675	-3.000e-06	0.00268	0.4	0.352
lieb_000_18691	BrCaNd ₃ Sn ₃	8	-3.516	-4.377	0.000e+00	0.0035	1.23	2.621
lieb_000_18708	AgDy ₄ Na ₂ Tl ₅	12	-2.79	-3.011	0.000e+00	0.00591	0.649	0.836
lieb_000_18772	Mg ₄ Sb ₃ Sn ₂ Tb ₃	12	-3.378	-3.654	-2.000e-05	0.00821	1.403	2.79
lieb_000_18796	Au ₄ I ₂ Nd ₃ Te ₃	12	-3.522	-4.06	-6.200e-05	0.00558	0.833	3.569
lieb_000_18819	AuGd ₅ IRu ₃ Se	11	-5.158	-5.8	4.000e-06	0.00626	1.197	2.65
lieb_000_18821	Ge ₂ Ni ₃ Tc ₃	8	-6.966	-7.062	-2.000e-06	0.0098	0.457	0.222
lieb_000_18831	Br ₈ Gd ₄	12	-4.235	-4.24	1.000e-06	0.00351	0.071	0.068
lieb_000_18841	Cs ₅ Yb ₃	8	-0.76	-0.895	8.000e-07	0.00296	2.487	2.77
lieb_000_18865	Gd ₄ MnSe ₇	12	-5.054	-5.609	-4.000e-06	0.00792	1.106	1.477
lieb_000_18899	LiP ₃ Rh ₂ Ru ₃ U ₂	11	-7.456	-7.989	3.000e-06	0.00596	0.585	0.598
lieb_000_18902	Co ₈	8	-6.744	-6.842	-8.000e-06	0.00869	0.166	0.185
lieb_000_18905	Br ₅ Tb ₃ V	9	-3.623	-4.258	-4.000e-06	0.0047	1.847	2.683
lieb_000_18912	CaEuNa ₅ SnTb ₃ Tl	12	-2.34	-2.511	1.000e-06	0.00725	0.847	1.097
lieb_000_18915	Ca ₃ Gd ₅ Sn ₄	12	-4.102	-4.125	-3.000e-06	0.00417	0.16	0.156
lieb_000_18920	CdGd ₅ Sn ₂	8	-4.117	-4.32	-1.000e-06	0.0037	0.647	0.393
lieb_000_18921	GeInNd ₄ ScSn ₄ Te	12	-4.382	-4.886	0.000e+00	0.00655	1.309	2.804
lieb_000_18927	Pt ₅ Ru ₃	8	-7.012	-7.209	-2.000e-06	0.00549	0.315	0.306
lieb_000_18933	Br ₄ KSbTb ₃	9	-3.028	-3.97	-9.000e-06	0.0095	2.068	3.914
lieb_000_18936	CdNa ₃ SrYb ₃	8	-1.282	-1.334	5.000e-06	0.00333	2.013	0.905
lieb_000_18956	Co ₂ Mn ₂ Ni ₄	8	-6.451	-6.592	-1.000e-06	0.0022	0.191	0.178
lieb_000_18972	Ga ₄ Li ₂ Nd ₃ SbZr ₂	12	-4.095	-4.579	-6.000e-06	0.00742	1.339	1.394
lieb_000_19009	Co ₅ PtSi ₂	8	-6.533	-6.724	-2.000e-06	0.00411	0.286	0.907
lieb_000_19043	RhRu ₃ Sn ₂ V ₃ Zn ₃	12	-5.668	-6.067	1.000e-06	0.00754	1.013	1.834
lieb_000_19065	Ga ₂ Pt ₃ Ru ₃	8	-6.599	-6.616	0.000e+00	0.00462	0.136	0.078
lieb_000_19075	GaN ₃ Nd ₃ Pb	8	-2.739	-3.159	-1.000e-06	0.00684	2.05	2.725
lieb_000_19098	Te ₄ TlYb ₃	8	-2.885	-3.666	-4.000e-06	0.00357	1.402	3.233
lieb_000_19143	Gd ₃ Na ₅	8	-2.168	-2.251	-5.000e-06	0.00504	1.362	2.899
lieb_000_19174	GaN ₇	8	-5.265	-5.268	-1.000e-06	0.00432	0.058	0.047
lieb_000_19193	AlCdDy ₅ PbReRh ₂	11	-5.122	-5.585	-4.000e-06	0.00952	1.241	2.687
lieb_000_19209	Ni ₃ Pt ₅	8	-5.774	-5.92	2.000e-06	0.00299	0.297	2.483
lieb_000_19232	Co ₃ FeNi ₈	12	-5.856	-5.951	0.000e+00	0.00621	0.326	0.209
lieb_000_19233	CdEu ₃ SnTb ₃	8	-3.055	-3.253	-2.000e-06	0.005	0.454	0.437
lieb_000_19234	Tl ₃ Yb ₅	8	-1.818	-2.1	6.000e-06	0.00375	1.201	0.515
lieb_000_19273	BaGd ₅ RhSn ₃ Sr ₂	12	-4.04	-4.284	0.000e+00	0.00404	0.629	3.612
lieb_000_19308	Gd ₃ Pt ₂ Ru ₃	8	-6.86	-7.046	-1.100e-05	0.00787	0.614	1.047
lieb_000_19309	I ₃ Nd ₃ TeTl	8	-3.575	-3.911	1.000e-06	0.004	1.368	1.467

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