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Received: 17 January 2024

Accepted: 10 January 2025

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Cite this article as: Zeni, C. et al. A generative model for inorganic materials design. *Nature* <https://doi.org/10.1038/s41586-025-08628-5> (2025)

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# A generative model for inorganic materials design

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## Abstract

The design of functional materials with desired properties is essential in driving technological advances in areas like energy storage, catalysis, and carbon capture [1–3]. Generative models provide a new paradigm for materials design by directly generating novel materials given desired property constraints, but current methods have low success rate in proposing stable crystals or can only satisfy a limited set of property constraints [4–11]. Here, we present MatterGen, a model that generates stable, diverse inorganic materials across the periodic table and can further be fine-tuned to steer the generation towards a broad range of property constraints. Compared to prior generative models [4, 12], structures produced by

MatterGen are more than twice as likely to be novel and stable, and more than 10 times closer to the local energy minimum. After fine-tuning, MatterGen successfully generates stable, novel materials with desired chemistry, symmetry, as well as mechanical, electronic and magnetic properties. As a proof of concept, we synthesize one of the generated structures and measure its property value to be within 20 % of our target. We believe that the quality of generated materials and the breadth of MatterGen’s capabilities represent a major advancement towards creating a foundational generative model for materials design.

## 1 Introduction

The rate at which we can discover better materials has a major impact on the pace of technological innovation in areas such as carbon capture, semiconductor design, and energy storage [1–3]. Traditionally, most materials have been discovered through experimentation and human intuition, limiting the number of candidates that can be tested and causing long iteration cycles. Thanks to the advance of high-throughput screening [13], open material databases [14–17], machine-learning-based property predictors [18, 19], and machine learning force fields (MLFFs) [20, 21], it has become possible to screen hundreds of thousands of materials to identify promising candidates [22, 23]. However, screening-based methods are still fundamentally limited by the number of known materials. The largest explorations of previously unknown crystalline materials are in the orders of  $10^6$ – $10^7$  materials [21, 23–25], which is only a tiny fraction of the number of potential stable inorganic compounds [26]. Moreover, these methods cannot be efficiently steered towards finding materials with target properties.

Given these limitations, there has been great interest in the inverse design of materials [27, 28]. The aim of inverse design is to directly generate material structures that satisfy target property constraints, e.g., via generative models [4, 8, 11], evolutionary algorithms [29], and reinforcement learning [30]. Generative models are promising since they can efficiently explore new structures and be flexibly adapted to different downstream tasks. However, current generative models often fall short of producing stable materials according to density functional theory (DFT) calculations [4, 5, 31], are constrained by a narrow subset of elements [7, 9], and/or can only optimize a very limited set of properties, mainly formation energy [4, 5, 8, 11, 31, 32].

In this study, we present MatterGen, a diffusion-based generative model that generates stable, diverse inorganic materials across the periodic table and can be fine-tuned towards a wide range of downstream tasks for inverse materials design (Fig. 1). To enable this, we introduce a diffusion process that generates crystal structures by gradually refining atom types, coordinates, and the periodic lattice. We further introduce adapter modules to enable fine-tuning on desired chemical composition, symmetry, and scalar property constraints like magnetic density. Compared to previous state-of-the-art generative models for materials [4, 12], MatterGen more than doubles the percentage of generated stable, unique, and novel (S.U.N.) materials, and generates structures that are more than 10 times closer to their ground-truth structures at the DFT local energy minimum (Fig. 2). MatterGen’s broad conditioning capabilities

**Fig. 1: Inorganic materials design with MatterGen.** (a) MatterGen generates stable materials by reversing a corruption process through iteratively denoising a random structure. The forward diffusion process independently corrupts atom types  $\mathbf{A}$ , coordinates  $\mathbf{X}$ , and the lattice  $\mathbf{L}$  towards a physically motivated distribution of random materials. (b) An equivariant score network is pre-trained on a large dataset of stable material structures to jointly denoise atom types, coordinates, and the lattice. The score network is then fine-tuned with a labeled dataset through an adapter module that adapts the model using the encoded property  $c$ . (c) The fine-tuned model generates materials with desired chemistry, symmetry, or scalar property constraints.

enable inverse materials design for a much wider range of problems than prior generative models. When fine-tuned, MatterGen often generates more S.U.N. materials in target chemical systems than well-established methods like substitution and random structure search (RSS) (Fig. 3), is capable of generating highly symmetric structures given desired space groups (Fig. D8), and directly generates S.U.N. materials that satisfy target mechanical, electronic, and magnetic property constraints (Fig. 4). MatterGen is also able to design materials given multiple property constraints, e.g., high magnetic density and a chemical composition with low supply-chain risk (Fig. 5). As a proof of concept, we validate MatterGen’s design capabilities by synthesizing a generated material and measuring its property to be within 20 % of our target (Fig. 6).

## 2 Results

### 2.1 Diffusion process for materials

MatterGen is a diffusion model tailored for designing crystalline materials across the periodic table (Fig. 1(a)). Diffusion models generate samples by reversing a fixed corruption process via a learned score network [33–35]. Corruption processes for images typically add Gaussian noise but crystalline materials have unique periodic structure and symmetries which demand a customized diffusion process. We define a crystalline material by its repeating unit, i.e., its unit cell, comprising the atom types  $\mathbf{A}$  (i.e., chemical elements), coordinates  $\mathbf{X}$ , and periodic lattice  $\mathbf{L}$  (Supplementary A.1 and A.2). For each component, we define a corruption process that considers its particular geometry and has a physically motivated limiting noise distribution. The coordinate diffusion respects the periodic boundary via a wrapped Normal distribution and approaches a uniform distribution at the noisy limit. We adjust for the effect of cell size on the fractional coordinate diffusion in Cartesian space by scaling the noise magnitude accordingly (Supplementary A.6). Our lattice diffusion takes a symmetric form and approaches a distribution whose mean is a cubic lattice with average atomic density from the training data (Supplementary A.7). Atom types are diffused in categorical space where individual atoms are corrupted into a masked state (Supplementary A.5). To reverse the corruption process, we learn a score network that outputs equivariant scores for atom types, coordinates, and lattice, removing the need to learn symmetries from data (Supplementary A.8 and A.9).

To design materials with desired property constraints, we introduce adapter modules for fine-tuning the score model on an additional dataset with property labels (Fig. 1(b), Supplementary B). The adapter modules are tunable components injected into each layer of the base model to alter its output depending on the given property label [36]. Fine-tuning is appealing as it still works well if the labeled dataset is small compared to unlabeled structure datasets, as is often the case due to the high computational cost of calculating properties. The fine-tuned model is used in combination with classifier-free guidance [37] to steer the generation towards target property constraints. We apply this approach to multiple types of constraints, producing a set of fine-tuned models that can generate materials with target chemical composition, symmetry, or scalar properties such as magnetic density (Fig. 1(c)). These broad conditioning capabilities combined with the improvements in the diffusion process over prior work [4, 12] are key for addressing a wide range of inverse design problems (Supplementary A.11).

## 2.2 Generating stable, diverse materials

We formulate learning a generative model for inverse materials design as a two-step process, where we first pre-train a general base model for generating stable, diverse crystals across the periodic table, and then we fine-tune this model towards different downstream tasks. To train the base model, we curate a large and diverse dataset, Alex-MP-20, comprising 607,683 stable structures with up to 20 atoms recomputed from the Materials Project (MP) [14] and Alexandria [25, 38] datasets (Supplementary C).

In this section, we focus on the ability of MatterGen’s base model to generate stable, diverse materials, which we argue is a prerequisite for addressing any inverse materials design task. Since diversity is difficult to measure directly, we resort to quantifying MatterGen’s ability to generate S.U.N. materials (Supplementary D.3), and provide an additional analysis of the quality and diversity of generated structures. We consider a structure to be stable if its energy per atom after relaxation via DFT is within 0.1 eV/atom above the convex hull defined by a reference dataset, Alex-MP-ICSD, comprising 850,384 unique structures recomputed from the MP [14], Alexandria [25, 38], and Inorganic Crystal Structure Database (ICSD) [39] datasets (Supplementary C). We consider a structure to be unique if it does not match any other structure generated by the same method. We consider a structure to be novel if it does not match any structure present in an extended version of Alex-MP-ICSD containing 117,652 disordered ICSD structures in addition to the 850,384 ordered structures used to compute the reference convex hull. To account for compositional disorder effects [40], we match structures based on a newly proposed ordered-disordered structure matcher (Supplementary D.4). We adopt these definitions throughout unless stated otherwise.

Fig. 2(a) shows several random samples generated by MatterGen, featuring typical coordination environments of inorganic materials; see Supplementary D.5.3 for a more detailed analysis. To assess stability, we perform DFT calculations on 1024 generated structures. Fig. 2(b) shows that 78 % of generated structures fall below the 0.1 eV/atom threshold (13 % below 0.0 eV/atom) of MP’s convex hull, while 75 % fall below the 0.1 eV/atom threshold (3 % below 0.0 eV/atom) of the combined Alex-MP-ICSD hull. Further, 95 % of generated structures have an RMSD w.r.t. their

**Fig. 2: Generating stable, unique and novel inorganic materials.** (a) Visualization of four randomly selected crystals generated by MatterGen, with corresponding reduced formula and space group. (b) Distribution of energy above hull values of generated structures using MP and Alex-MP-ICSD datasets as energy references, respectively. (c) Distribution of root mean squared displacement (RMSD) between initial generated and DFT-relaxed structures. (d) Percentage of unique, novel structures as a function of number of generated structures. (e-f) Percentage of S.U.N. structures (e) and average RMSD between initial and DFT-relaxed structures (f) for MatterGen, MatterGen-MP and several baseline models, including DiffCSP [12], CDVAE [4], P-G-SchNet, G-SchNet [41], and FTCP [31]. Training datasets are in parentheses.

DFT-relaxed structures that is below 0.076 Å (Fig. 2(c)), which is almost one order of magnitude smaller than the atomic radius of the hydrogen atom (0.53 Å). These results indicate that the majority of structures generated by MatterGen are stable, and very close to the DFT local energy minimum.

We further investigate whether MatterGen can generate a substantial amount of unique and novel materials. We find that the percentage of unique structures is 100 % when generating 1000 structures and only drops to 52 % after generating ten million structures, while 61 % of generated structures are novel (Fig. 2(d)). This suggests that MatterGen is able to generate diverse structures without significant saturation even at a large scale, and that the majority of those structures are novel w.r.t. Alex-MP-ICSD. Remarkably, we also find that MatterGen has re-discovered more than 2000 experimentally verified structures from ICSD not seen during training (Supplementary D.5.4), showing its ability to generate synthesizable materials.

Next, we benchmark MatterGen against previous generative models for materials and show a significant performance improvement. We focus on two metrics averaged over 1000 generated samples from each method: (1) the percentage of S.U.N. materials among generated samples, measuring the success rate of generating promising candidates, and (2) the average RMSD between generated samples and their DFT-relaxed structures, measuring the distance to equilibrium (Supplementary D.5.1). We also compare to MatterGen-MP, which is a MatterGen model trained only on MP-20, i.e., the same, smaller, dataset used by the other baselines. Compared to the previous state-of-the-art methods CDVAE [4] and DiffCSP [12], MatterGen-MP generates 60 % more S.U.N. structures while the average RMSD of the generated structures is 50 % lower (Fig. 2(e-f)). We find that our model design choices are crucial for the improved performance (Supplementary A.10). When comparing MatterGen with MatterGen-MP, we observe a further 70 % increase in the percentage of S.U.N. structures and a five times decrease in RMSD as a result of scaling up the training dataset.

Combining both model and data improvements, MatterGen generates structures that are more than twice as likely to be S.U.N. compared to previous generative models while the generated structures are up to an order of magnitude closer to their local energy minimum. Next, we fine-tune the pre-trained base model of MatterGen towards different downstream applications, including target chemistry (Section 2.3) and scalar property constraints (Sections 2.4 and 2.5), with additional experimental validation

**Fig. 3: Generating materials in target chemical system.** (a-b) Mean percentage of S.U.N. structures generated by MatterGen and baselines for 27 chemical systems, grouped by system type (a) and number of elements (b). Error bars denote 95 % percentile intervals ( $n=9$ ). (c-d) Number of structures on the combined convex hull found by each method and in the Alex-MP-ICSD dataset, grouped by system type (c) and number of elements (d). (e) Convex hull diagram for V-Sr-O, a well-explored ternary system. Dots denote structures on the hull, their coordinates show the element ratio of their composition, and their color indicates by which method they were discovered. (f-i) Four structures MatterGen discovered (re-discovered in the case of (f)) on the V-Sr-O hull depicted in (e), along with their reduced formula and space group.

in Section 2.6. Results for fine-tuning on symmetry constraints are in Supplementary D.7.

### 2.3 Chemistry-guided design

Finding the most stable material structures in a target chemical system (e.g., Li-Co-O) is crucial to define the true convex hull required for assessing stability, and indeed is one of the major challenges in materials design [42]. The most comprehensive approach for this task is *ab initio* RSS [43], which has been used to discover many novel materials that were later experimentally synthesized [42]. The biggest drawback of RSS is its computational cost, as the thorough exploration of even a ternary compound can require hundreds of thousands of DFT relaxations. In recent years, the combination of generating structures via RSS, substitution or evolutionary methods with MLFFs has proven successful in exploring chemical systems [21, 23, 44].

Here, we evaluate MatterGen’s ability to explore target chemical systems by comparing it with substitution and RSS. We equip all methods with the MatterSim [45] MLFF to pre-relax and filter the generated structures by their predicted stability before running more expensive DFT calculations. We fine-tune the MatterGen base model (Supplementary B.1) and steer the generation towards different target chemical systems and an energy above hull of 0.0 eV/atom. We evaluate the methods on nine ternary, nine quaternary, and nine quinary chemical systems. For each of these three groups, we pick three chemical systems at random from the following categories: well explored, partially explored, and not explored (Supplementary D.6).

MatterGen generates the highest percentage of S.U.N. structures for every system type and every chemical complexity (Fig. 3(a-b)). In addition, MatterGen finds the highest number of unique structures on the combined convex hull in (1) ‘partially explored’ systems, where existing known structures near the hull were provided during training, and in (2) ‘well-explored systems’, where structures near the hull are known but were not provided in training (Fig. 3(c)). While substitution offers a comparable or more efficient way to generate structures on the hull for ternary and quaternary systems, MatterGen achieves better performance on quinary systems (Fig. 3(d)). Remarkably, the strong performance of MatterGen in quinary systems was achieved with only 10,240 generated samples, compared to  $\sim$ 70,000 samples for substitution and 600,000 for RSS. This underscores the enormous efficiency gains that can

**Fig. 4: Designing materials with target magnetic, electronic, and mechanical properties.** (a-c) Density of property values among (1) S.U.N. samples generated by MatterGen, and (2) structures in the labeled fine-tuning dataset for a magnetic, electronic, and mechanical property, respectively. The property target for MatterGen is shown as a black dashed line. Magnetic density values  $< 10^{-3} \text{ \AA}^{-3}$  in (a) are excluded from the labeled data to improve readability. (d-f) Visualization of S.U.N. structures with the best property values generated by MatterGen for magnetic density (d), band gap (e), and bulk modulus (f), along with their reduced formula, space group, and property value. (g-h) Number of S.U.N. structures that satisfy target constraints found by MatterGen and baselines across DFT property calculation budgets.

be realized with generative models by proposing better initial candidates. Finally, we show that MatterGen finds three novel (four overall) structures on the combined hull for V-Sr-O—an example of a well-explored ternary system—while substitution finds three (five overall), and RSS only one (two overall) (Fig. 3(e)). Structures discovered by MatterGen are shown in Fig. 3(f-i), and are analyzed in Supplementary D.6.2.

## 2.4 Property-guided design

There is an enormous need for materials with improved properties across many applications, including energy storage, catalysis, and carbon capture [1–3]. The classical screening-based approach starts from a set of candidates and selects the ones with the best predicted properties, but screening cannot explore structures beyond the set of known materials. Here, we demonstrate MatterGen’s ability to directly generate S.U.N. materials with target constraints on three different inverse design tasks, featuring a diverse set of properties—magnetic, electronic, and mechanical—with varying degrees of available labeled data for fine-tuning the model. In the first task, we aim to generate materials with high magnetic density, a prerequisite for permanent magnets. We fine-tune the model on 605,000 structures with DFT magnetic density labels (calculated assuming ferromagnetic ordering) and generate structures with a target magnetic density value of  $0.20 \text{ \AA}^{-3}$ . Second, we fine-tune the model on 42,000 structures with DFT band gap labels and sample materials with a target band gap value of 3.0 eV. Finally, we target structures with high bulk modulus—an important property for superhard materials. We fine-tune the model on only 5,000 labeled structures, and sample with a target value of 400 GPa. While these tasks were chosen to evaluate the model’s generality, further investigations would be required to assess the suitability of these materials for specific applications, e.g., a superhard material needs to have a high shear modulus, and a permanent magnet needs a suitable magnetic order and critical temperature. Further experimental details are in Supplementary D.8.

In Fig. 4(a-c), we observe a significant shift in the distribution of property values among S.U.N. samples generated by MatterGen towards the desired targets, even when the targets are at the tail of the data distribution. This still holds true for properties where the number of DFT labels available for fine-tuning the model is substantially smaller than the size of the unlabeled training data. In Fig. 4(d-f) we depict the S.U.N.

structures with the best predicted property values generated by MatterGen for each task, with additional analysis in Supplementary D.8.2.

Moreover, we assess how many S.U.N. structures satisfying extreme property constraints can be found by MatterGen when given a limited budget for DFT property calculations. As a baseline, we count the number of materials in the labeled fine-tuning dataset that satisfy the constraint. We also compare with a screening approach, which scans previously unlabeled materials for promising candidates. In contrast to the previous experiment, we fine-tune MatterGen with labels predicted by a machine learning property predictor—the same used for the screening baseline—when the dataset is not fully labeled. MatterGen is able to find up to 18 S.U.N. structures with magnetic density above  $0.2 \text{ \AA}^{-3}$  using only 180 DFT property calculations (Fig. 4(g)). Since the dataset is fully labeled, there is no screening baseline available. MatterGen also finds substantially more S.U.N. materials with high bulk modulus than screening (Fig. 4(h)). While the number of structures found by screening saturates with increasing budget, MatterGen keeps discovering S.U.N. structures at an almost constant rate. Given a budget of 180 DFT property calculations, we find 106 S.U.N. structures (with 95 distinct compositions), more than double the number found with a screening approach (40, 28 distinct compositions). In contrast, there are only two materials in the labeled fine-tuning dataset with such high bulk modulus values. Note that both MatterGen and screening produce multiple structures per chemical system that are unique according to our definition (Supplementary D.4) but could potentially be alloys with different stoichiometries [40].

## 2.5 Designing low-supply-chain-risk magnets

Most materials design problems require finding structures satisfying multiple property constraints. While MatterGen can be fine-tuned for any combination of constraints, here we focus on designing low-supply-chain-risk magnets. Since many existing high-performing permanent magnets contain rare earth elements that pose supply chain risks, there has been increasing interest in discovering rare-earth-free permanent magnets [46]. We simplify this task to finding materials with a high magnetic density of  $0.2 \text{ \AA}^{-3}$  and a low Herfindahl–Hirschman index (HHI) score of 1250, where a material with an HHI score below 1500 is considered to have low supply chain risk [47] (experimental details in Supplementary D.9.1); in practice, additional properties like high coercivity, suitable magnetic order and critical temperature need to be satisfied.

**Fig. 5: Designing low-supply-chain-risk magnets.** (a) Distribution of S.U.N. structures generated by MatterGen when fine-tuned on the HHI score (single) and on both HHI score and magnetic density (joint), as well as structures from the labeled fine-tuning dataset. MatterGen’s property target is shown as a black cross. (b) Occurrence of most frequent elements in S.U.N. structures for the two fine-tuned MatterGen models. (c) S.U.N. structures on the Pareto front for the jointly fine-tuned model, along with their reduced formula, space group, magnetic density, and HHI score.

In Fig. 5(a), we observe that MatterGen generates S.U.N. structures that are narrowly distributed around the target values, despite the labeled fine-tuning data being extremely scarce in that region. Compared to a model that only targets high magnetic density values (single), targeting both properties (joint) shifts the distribution of HHI scores closer towards the desired target value while retaining high magnetic density values. Due to the lower HHI scores, elements often found in magnets that have supply chain issues, e.g., Cobalt (Co) and Gadolinium (Gd), have been almost completely eliminated from the structures generated by the jointly fine-tuned model (Fig. 5(b)). We show some of these structures in Fig. 5(c) and analyze them in more detail in Supplementary D.9.2. Finally, we find that MatterGen has re-discovered 67 previously synthesized, disordered structures from ICSD that were unseen during training, many of which are similar to known permanent magnetic materials (Supplementary D.9.3).

## 2.6 Experimental validation

As a proof of concept, we experimentally synthesize a material designed by MatterGen and show that the experimentally measured property is close to our design target. We generate 8192 candidates using a model fine-tuned on bulk modulus for each of the four target bulk modulus values: 50, 100, 150, and 200 GPa (Supplementary D.10.1). We perform multiple rounds of filtering based on (1) uniqueness and novelty, (2) energy above the hull stability from MatterSim [45] and DFT, (3) phonon stability from MatterSim [45], and (4) whether the material contains oxygen (Supplementary D.10.3). The filtering narrows the number of candidates down to 75, from which we select four for experimental synthesis after expert inspection. Synthesis was successful for one of the four candidates (Supplementary D.10.4 and D.10.5). According to the Rietveld refinement analysis, the synthesized material is  $TaCr_2O_6$ , a compositionally disordered version of the ordered structure predicted by MatterGen (Fig. 6(a-c), Supplementary D.10.6). This structure was generated by targeting a bulk modulus value of 200 GPa; we predict a value of 222 GPa using DFT for the ordered  $TaCr_2O_6$  structure generated by MatterGen, and similar bulk modulus values (219 GPa) for two other ordered approximations corresponding to the same disordered structure (Fig. 6(c)). We also experimentally measure the sample's Young's modulus via nanoindentation, and estimate its bulk modulus using the DFT-computed Poisson ratio of 0.30. The estimated bulk modulus is up to 169 GPa after four measurements ( $158 \pm 11$  GPa), where the maximum of the four measurements is our best estimate given that the experimental powder sample is likely non-compact (Supplementary D.10.8).

By examining the original 8192 samples generated for each of the four target values, we find that MatterGen has re-discovered experimentally verified ICSD compounds not present in our training set (Supplementary D.10.2). We identify 101 matches according to our ordered-disordered structure matcher (Supplementary D.4), and successfully compute DFT bulk modulus values for 95 of them (Fig. 6(d)). The DFT-computed values align well with the target values used for conditional generation, with a mean absolute error of 23 GPa and a root mean squared error of 32 GPa.

**Fig. 6: Experimental validation of generated structures.** (a) Rietveld refinement for the experimental sample we synthesize, including the measured x-ray diffraction (XRD) spectra (yellow dots), the theoretical fit (black line), and the difference between the two (teal line). Vertical ticks (purple) highlight the major peaks of  $TaCr_2O_6$  and  $Cr_2O_3$ . A picture of the sample is included. (b) Two views of the  $TaCr_2O_6$  structure generated by MatterGen that we use as a synthesis target, along with the reduced formula, space group, and DFT bulk modulus value. (c) Two views of the disordered  $TaCr_2O_6$  structure we experimentally synthesize. (d) DFT bulk modulus values of structures generated by MatterGen that match experimentally verified ICSD structures not present in the training dataset, across four different target bulk modulus values. The yellow triangle indicates the generated structure from (b).

### 3 Discussion

Generative models are promising for tackling inverse design tasks as they can efficiently explore novel structures with desired properties. However, generating the 3D structure of stable crystalline materials is challenging due to their periodicity and the interplay between atom types, coordinates, and lattice. MatterGen improves upon limitations of previous methods by introducing a joint diffusion process for atom types, coordinates, and lattice, which—combined with a substantially larger training dataset—drastically increases the stability, uniqueness, and novelty of generated materials. MatterGen can be fine-tuned to generate S.U.N. structures satisfying target constraints across a wide range of properties, with performance improvements over widely-employed methods such as MLFF-assisted RSS and substitution, as well as ML-assisted screening. We verified that MatterGen is able to generate synthesizable structures by experimentally synthesizing a sampled structure and by re-discovering previously synthesized materials that were unseen by the model.

Despite these advances, MatterGen could still be improved in several ways. For example, we observe that the model disproportionately generates structures with P1 symmetry compared to the training data, indicating a tendency for generating less symmetric structures, especially for larger crystals (Supplementary D.2). We hypothesize that further improvements on the denoising process, the backbone architecture, and the expansion of the training dataset could enable the model to overcome such issues. We also acknowledge that our evaluations only cover some of the criteria required for real-world applicability, with experimental validation and characterization being the ultimate test [40]. We discuss challenges in evaluating the quality of crystalline materials from generative models in Supplementary D.2.

We believe that the breadth of MatterGen’s capabilities and the quality of generated materials represent a major advance towards creating a universal generative model for materials. Given the enormous impact of generative models in domains like image generation [48] and protein design [49], we envision that models like MatterGen will equally transform materials design in the coming years. As such, we are excited about the many directions in which MatterGen could be extended. For instance, MatterGen could be expanded to cover a broader class of materials ranging from catalyst surfaces to metal organic frameworks, enabling us to tackle challenging problems

like nitrogen fixation [50] and carbon capture [3]. The property constraints can be extended to non-scalar quantities like the band structure or XRD spectrum, which would enable applications ranging from band engineering to the prediction of atomic structures of experimentally-measured XRD spectra of unknown samples.

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## Data availability

Alex-MP datasets for training and fine-tuning the MatterGen model are available at <https://github.com/microsoft/mattergen>, along with CIF files for crystal structures presented in the manuscript, load-depth profiles for nanoindentation measurements, the measured XRD profile, and the Rietveld refinement for the TaCr<sub>2</sub>O<sub>6</sub> sample. MP structures (v2022.10.28) are from <https://materialsproject.org> and Alexandria structures are from <https://doi.org/10.24435/materialscloud:m7-50>, both under CC BY 4.0 license. Identifiers of ICSD structures (release 2023.1) used as part of our test set are provided in the Supplementary Information; structures are available at <https://icsd.products.fiz-karlsruhe.de> under a commercial license.

## Code availability

Source code for MatterGen is available at <https://github.com/microsoft/mattergen>.

**Acknowledgments** We thank our colleagues from Microsoft Research AI for Science for their contributions and support, including Andrew Foong, Bas Veeling, Yu Xie, Karin Strauss, Keqiang Yan, Cristian Bodnar, Rianne van den Berg, Frank Noé, Marwin Segler, Elise van der Pol, Max Welling, Rachel Howard, Tie-Yan Liu, Bonnie Kruft, and Chris Bishop; the Microsoft Azure Quantum team including Chi Chen, Leopold Talirz and Nathan Baker, the Materials Project team, and Chris Pickard for providing feedback; and the AI on Xbox team for providing part of the compute.

**Author contributions** AF, MH, RP, RT, TX, CZ and DZ (alphabetically ordered) conceived the study, implemented the methods, performed computational experiments, and wrote the manuscript. XF led the development of the adapter modules. ZW, CY, WL led the experimental synthesis and characterizations. AS implemented and ran the symmetry conditioned generation. JS implemented the band gap workflow. BN proposed the task of low-supply-chain risk magnets. ZL, YZ, HY, HH, and JL developed the machine learning force field. XF, SS, JC, LS, JS, BN, HS, SL, C-WH, ZL, YZ, HY, HH, and JL helped with implementing the methods, conducting computational experiments, and writing the manuscript. SU and RS acted as project managers. TX and RT led the research.

**Competing interests** AF, MH, RP, RT, TX, CZ and DZ are inventors of the pending, non-provisional patent application 18/759,208 in the name of Microsoft Technology Licensing LLC, relating to generative models for the computational design of materials. The other authors declare no competing interests.

## Additional information

**Supplementary information** is available for this paper.

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