MatterChat: A Multi-Modal LLM for Material Science

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Abstract

Understanding and predicting the properties of inorganic materials is crucial for accelerating advancements in materials science and driving applications in energy, electronics, and beyond. Integrating material structure data with language-based information through multi-modal large language models (LLMs) offers great potential to support these efforts by enhancing human–AI interaction. However, a key challenge lies in integrating atomic structures at full resolution into LLMs. In this work, we introduce MatterChat, a versatile structure-aware multi-modal LLM that unifies material structural data and textual inputs into a single cohesive model. MatterChat employs a bridging module to effectively align a pretrained machine learning interatomic potential with a pretrained LLM, reducing training costs and enhancing flexibility. Our results demonstrate that MatterChat significantly improves performance in material property prediction and human-AI interaction, surpassing general-purpose LLMs such as GPT-4. We also demonstrate its usefulness in applications such as more advanced scientific reasoning and step-by-step material synthesis.

Keywords: Foundation model, Large Language Model, Multi-Modal Learning, Inorganic Material

1 Introduction

In-silico material discovery and design have traditionally relied on high-fidelity first-principles methods such as density functional theory (DFT) [1] and ab-initio molecular dynamics (AIMD) [2] to accurately model atomic interactions and predict material properties. Despite their effectiveness, these methods face significant challenges due to their prohibitive computational cost, limiting their scalability for high-throughput screening across vast chemical spaces and for simulations over large length and time scales. Moreover, many advanced materials remain beyond the reach of widespread predictive theories due to a fundamental lack of mechanistic understanding. These challenges stem from the inherent complexity of their chemical composition, phase stability, and the intricate interplay of multiple order parameters, compounded by the lack of self-consistent integration between theoretical models and multi-modal experimental findings. As a result, breakthroughs in functional materials, such as new classes of correlated oxides, nitrides, and low-dimensional quantum materials, have largely been serendipitous or guided by phenomenological intuition rather than systematic, theory-driven design. Attempts to predict new materials and functionalities have often led to mixed results, with theoretically proposed systems failing to exhibit the desired properties when synthesized and tested. Achieving reliable, scalable, and predictive design of materials requires a paradigm shift.

With the rise of artificial intelligence (AI) in materials science, there has been a surge of methods aiming to overcome these limitations, ranging from machine learning (ML) surrogate models [3, 4], ML interatomic potentials (MLIPs) [5–7], and generative models [8, 9]. These models enable rapid predictions, accelerate large-scale simulations, and facilitate the generation of novel materials. As a result, they have significantly advanced fields such as energy storage [10], electronics [11], catalysis [12], and biomedical applications [13]. Among these promising ML approaches, graph-based models in material science have become increasingly popular due to their versatile graph representation of atomistic systems, where each atom is represented as a node, and chemical bonds to neighboring atoms are represented as edges. Although these graph-based methods have shown success in accurately predicting material properties, they typically lack the capacity to handle tasks that require understanding scientific context, literature-based insights, and domain-specific language [14]. In particular, these models do not support human–AI interaction through user prompts or textual descriptions, making it difficult to incorporate expert domain knowledge and user-specified requests to close the feedback loop.

This bottleneck has inspired a wave of exploration into how natural language processing (NLP), and particularly large language models (LLMs), might be leveraged to fill the gap. LLMs like BERT [15], GPT [16], and newer open-source LLMs such as Mistral [17], Llama [18] and DeepSeek [19] have shown substantial promise across different domains by interpreting and generating language. Trained on extensive datasets, these models can support some scientific tasks that require interpretive language capabilities, such as question-answering (QA) [20] and retrieving information from unstructured text sources [21]. In recent years, there has been several efforts incorporating LLM to solve material related problems [22, 23], either by leveraging pretrained LLMs or multi-modal LLMs. Unfortunately, these approaches rely on text-based representations, such as chemical formula [22], Simplified Molecular Input Line Entry System (SMILES) strings [23, 24], textual descriptions [25], or Crystallographic Information File (CIF) [26], which lose the full resolution of atomic structures. Consequently, they exhibit inferior performance compared to pure graph-based models for predicting material properties [25], and they also potentially hinder other downstream tasks where structural information is crucial. Thanks to the steady development of MLIPs [5–7], particularly in their universal form (uMLIPs) [7], these models can now serve as atomistic pre-trained models capable of supporting a wide range of applications. The locality assumption underlying uMLIPs ensures that they effectively represent the local environment of each atom. Therefore, it is feasible to extract structural information from atom embeddings in a pretrained uMLIP.

In this work, we present MatterChat, a multi-modal large language model designed for materials science. MatterChat integrates material structure data with textual user queries, combining insights from materials science and NLP. It enhances the capabilities of large language models by overcoming their traditional limitations in quantitative predictions and improving the handling of scientific material-related tasks, as demonstrated through comparisons with other LLMs. MatterChat also maintains robust human–AI interaction capabilities, offering an intuitive interface for complex queries, compared to physical ML models. Furthermore, by leveraging deep, embedded knowledge from state-of-the-art pretrained LLMs, MatterChat enables advanced scientific reasoning and synthesis process guidance. The embedding visualization analysis indicates that MatterChat effectively preserves structure and property information.

This has guided the adoption of a multi-modal Retrieval-Augmented Generation (RAG) approach that can enhance MatterChat's robustness during material task inference.

2 Results

2.1 Overview of MatterChat

Figure 1(a) presents the architecture of MatterChat, designed to process both material structures and user requests as inputs to generate text-based outputs for tasks such as material property prediction, structural analysis, and descriptive language generation. MatterChat consists of three core components: the Material Processing Branch, the Language Processing Branch, and the Bridge Model. The Material Processing Branch extracts atomic-level embeddings from material structures represented as graphs. These embeddings are then processed by the Bridge Model, which employs trainable queries to produce language model-compatible embeddings. Finally, the Language Processing Branch processes the user's text-based prompt (e.g., "What is the formation energy of the material?") into language embeddings. These embeddings are then combined with the query embeddings generated by the Bridge Model and fed into the LLM to produce the final output in text format. Below, we provide the details of each component.

Material Structure Branch. The Material Structure Branch encodes material structures as graphs that capture the atomic local environment. To process these graphs, we use CHGNet [27], a state-of-the-art graph-based uMLIP model designed for crystal structures, to process these graphs. CHGNet is pretrained on a diverse dataset of materials, encompassing a wide range of symmetries, compositions, and bonding types, enabling it to effectively model complex atomic interactions and structural details. By capturing essential compositional features, such as atomic types and chemical bonds, along with spatial features like bond angles, CHGNet generates high-quality atom embeddings that are both physically meaningful and well-suited for downstream tasks.

Language Branch. The language branch is used to process user's text-based prompts, such as requests for property predictions, chemical formulas, space group information, or other material characteristics. We use the Mistral 7B LLM [17], one of the latest open-source LLMs, chosen for its exceptional performance across a wide range of scientific and non-scientific tasks. This branch processes each prompt, transforming it into dense embeddings that capture the semantic content of the inquiry. These embeddings are then combined with the query embeddings processed by the bridge model using a structured fusion approach, allowing the model to effectively incorporate both textual and material information. This integration enables the LLM to generate precise and contextually relevant responses tailored to the user's specific material-related prompts.

Bridge Model. To facilitate the integration between atom embeddings and the language branch, we developed a bridge model inspired by the BLIP2 architecture [28], based on a multi-layer transformer framework. This bridge model includes 32 trainable query vectors that interact with atom embeddings using an alternating attention mechanism. Cross-attention in even-numbered layers extracts key features from the atom embeddings, while self-attention in odd-numbered layers enhances representational depth. This approach refines the atom embeddings into query embeddings that are most connected to text, as shown in Figure 1a. Finally, these refined representations are mapped to LLM-compatible embeddings via a linear projection layer.

Figure 1(b)-(c) provide an overview of the dataset of crystalline structures used in our training set. Figure 1(b) visualizes the material distribution on the periodic table, highlighting that the dataset evenly spans a diverse range of elements up to Plutonium. Figure 1(c) depicts the distribution of crystalline structures by space group across the dataset. The dataset was curated from the Materials Project [29] and contains 142,899 material structures. For each structure, we generated a corresponding text-based dataset encompassing 12 tasks: 3 descriptive tasks (chemical formula, space group, and crystal system) and 9 property prediction tasks. These property prediction tasks include metallicity, direct bandgap, stability, experimental observation (Exp Ob), magnetic status (Is Magnetic), magnetic order, formation energy, energy above the hull, and bandgap, as summarized in Figure 1(a). Further details regarding the training scheme, hyper-parameters, and dataset curation are provided in the Methods section.

2.2 Multi-modal Material task interactions with MatterChat

Figure 2 illustrates the human-AI interaction examples with MatterChat, across a diverse range of material property prediction and analysis tasks. The figure shows MatterChat's ability to effectively address

a broad spectrum of user prompts ranging from fundamental material attributes (e.g., chemical formulas, space groups and crystal system) to complex material properties (e.g., thermal stability, bandgaps, formation energies and energy above the hull). The top panels in Figure 2 shows three interactive examples of material property prompts from randomly selected materials from the Material Project Dataset. The top left panel presents a human-AI query interface with MatterChat for the material identified by ID "mp-1001021". It provides a detailed profile including the chemical formula $Y_2Zn_4Se_2$, its crystalline structure denoted by the space group Fd-3m, and electronic properties such as a bandgap of 0.21350 eV. The interface also addresses the material's lack of thermal stability. The top mid panel shows the interaction example with the material with mp ID of "mp-1028281". It provides a comprehensive breakdown of the material's composition attributes, including its chemical formula (Mg14V4Sb) and its space
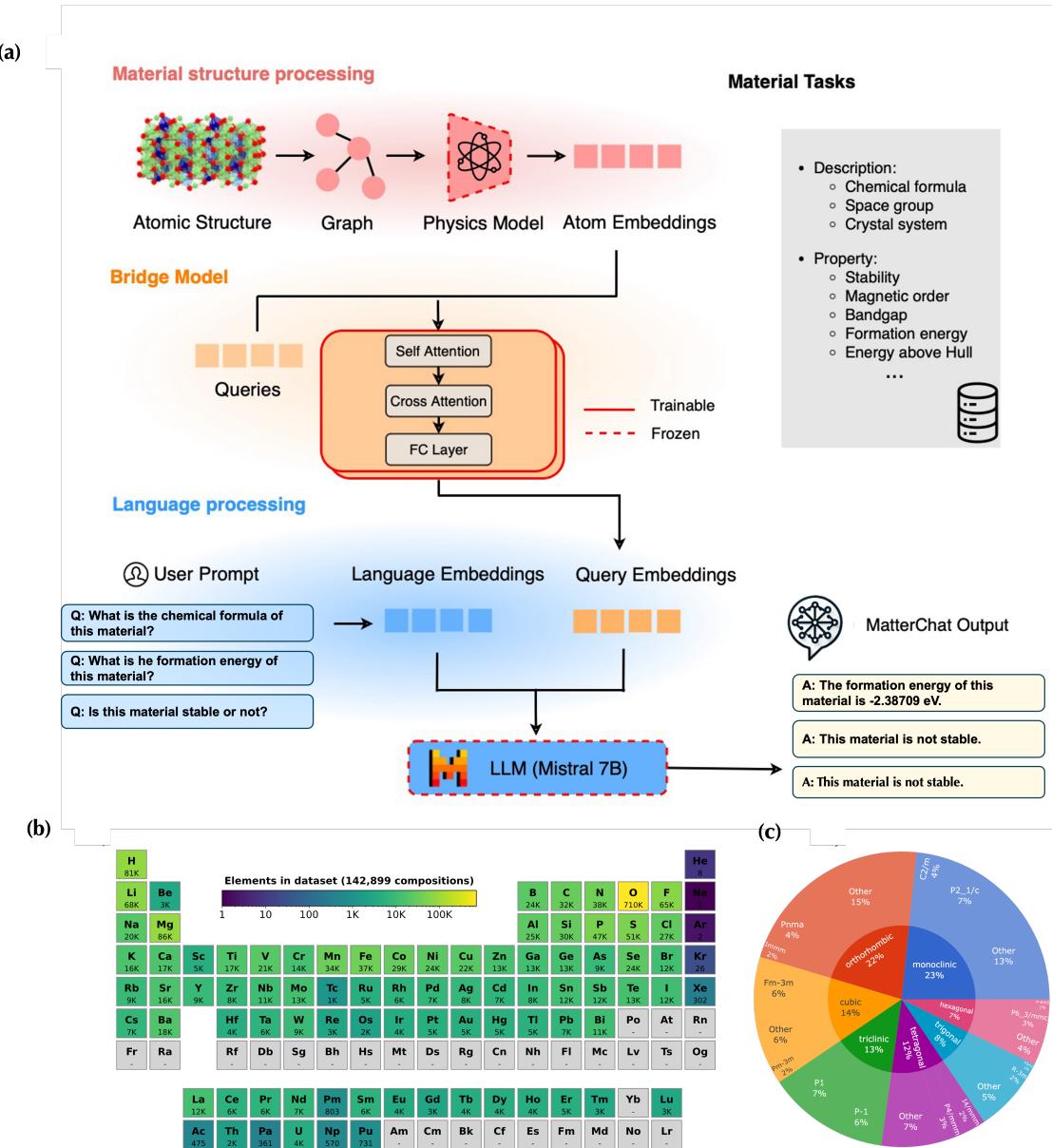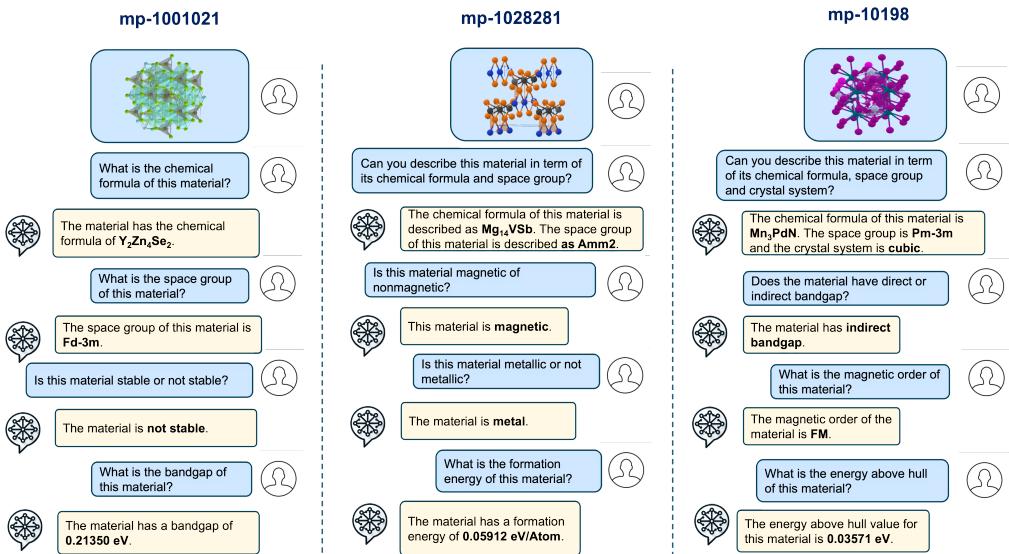
Fig. 1 Overview of MatterChat: a modular multi-modal LLM for material-based question-answering. (a) MatterChat architecture: The system includes a material encoder that generates atom embeddings and a LLM that processes language data. These components are connected by a trainable bridge model, which aligns material structure with natural language to support tasks such as material description and property prediction. (b) Elemental distribution across 142,899 compositions, representing the dataset's compositional diversity. (c) Dataset distribution shown by space groups (outer ring) and crystal Systems (inner ring), illustrating structural variation within the dataset.

(a) MatterChat interaction examples on material properties

mp-1001021

What is the chemical formula of this material?

The material has the chemical formula of $Y_2Zn_4Se_2$.

What is the space group of this material?

The space group of this material is Fd-3m.

Is this material stable or not stable?

The material is **not stable**.

What is the bandgap of this material?

The material has a bandgap of **0.21350 eV**.

mp-1028281

Can you describe this material in term of its chemical formula and space group?

The chemical formula of this material is described as $Mg_{14}VSb$. The space group of this material is described as Amm2.

Is this material magnetic of nonmagnetic?

This material is **magnetic**.

Is this material metallic or not metallic?

The material is **metal**.

What is the formation energy of this material?

The material has a formation energy of **0.05912 eV/Atom**.

mp-10198

Can you describe this material in term of its chemical formula, space group and crystal system?

The chemical formula of this material is Mn_3PdN. The space group is **Pm-3m** and the crystal system is **cubic**.

Does the material have direct or indirect bandgap?

The material has **indirect bandgap**.

What is the magnetic order of this material?

The magnetic order of the material is **FM**.

What is the energy above hull of this material?

The energy above hull value for this material is **0.03571 eV**.

(b) Formation energy prediction between MatterChat and other LLMs on new discovered materials

Ground Truth: **-0.098 eV/atom.**

mp-3202380

Gemini: Ef(Cd2Sb2Pb) ≈ **-0.28 eV/atom.**

This compound is likely to have a formation formation energy around **-0.75 eV/atom.**

deepseek: Estimated Formation Energy: ΔH_f ≈ **-0.44 eV/atom.**

The formation energy of this material is **-0.04389 eV/Atom.**

Ground Truth: **-0.563 eV/atom.**

mp-3206774

Gemini: The estimated formation formation energy is around **-8.18 eV per atom.**

This compound is likely to have a formation formation energy around **-6.04 eV per atom.**

deepseek: The formation energy value is ≈ **-1.83 eV/atom.**

The bandgap of the material is **-0.57142 eV/Atom.**

Fig. 2 MatterChat accurately predicts material properties accurately and outperforms the state-of-art LLMs. (a) Illustration of multi-modal material property queries using MatterChat. The model accurately interprets user prompts to predict chemical formulas, crystallographic properties, stability, electronic bandgap, magnetic order, and energy metrics of materials. The three panels demonstrate the framework's ability to address diverse material science inquiries, showing its alignment of graph-based and textual embeddings for precise question answering. (b) Comparative evaluation of formation energy predictions for newly discovered material from GNoME [30]. Predictions from Matterchat compared against the ground truth values along with evaluations from commerical LLMs (Gemini [31], GPT-4o [32] and DeepSeek [19]). The results show the accuracy and stability of the Matterchat in quantitative material evaluation tasks, which closely aligns with the ground truth, demonstrating its ability to integrate material graph embeddings for precise property prediction.

group (Amm2). The interaction further predicts that the material is both magnetic and metallic, and its formation energy is estimated at 0.05912 eV/atom. The top right panel provides an interaction example with MatterChat of the material with Materials Project ID of "mp-10198". This panel informs user's query about the chemical composition Mn3PdN and its cubic crystal structure, with the space group classified as Pm-3m. Additionally, it estimated that the material possesses an indirect bandgap, which is an important characteristic for applications in electronics. MatterChat also accurately predicts the ferromagnetic (FM) magnetic behaviors that the material exhibits, and it mentions its energy above hull value at 0.03571 eV. In the bottom panel, we present a comparative evaluation of MatterChat's performance on formation energy evaluation tasks for newly discovered materials from GNoME [30]. The model was compared against commercial LLMs, Gemini [31], GPT-4o [32] and DeepSeek [19]. The results show MatterChat's superior accuracy in estimating formation energies, consistently delivering predictions closer to the ground truths. For example, MatterChat's formation energy predictions for "mp-3202380" and "mp-3206774" show a remarkable alignment with the ground truth values. These results demonstrate MatterChat's ability to integrate structural and textual data seamlessly for a wide range of material property tasks.
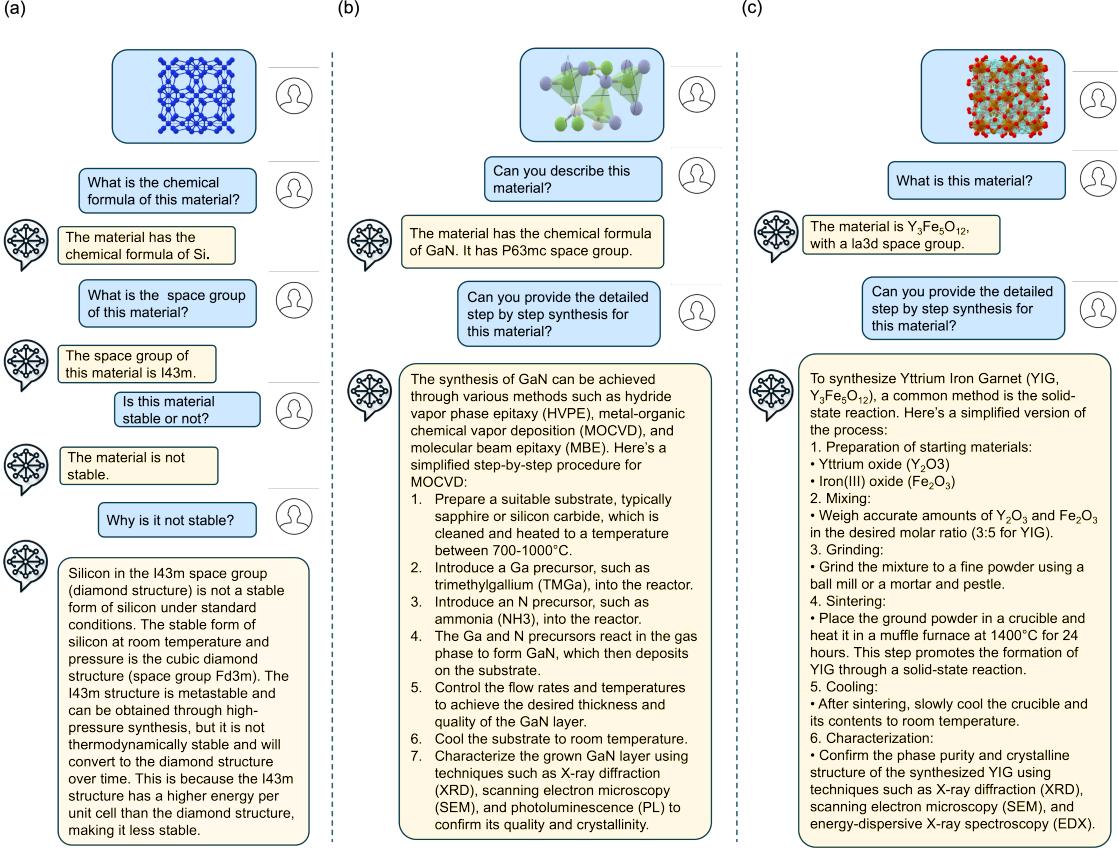
Fig. 3 MatterChat has the ability to solve more sophisticated tasks inherited from the pretrained LLM.
(a) Material property query for silicon (Si), including its chemical formula, space group, stability, and the reasoning for why it is not stable under standard conditions. (b) Highlights a material query for Gallium Nitride (GaN), providing its chemical formula, space group, and a step-by-step synthesis procedure using methods like HVPE, MOCVD, and MBE. (c) Material query interaction, Yttrium Iron Garnet (YIG, $Y_3Fe_5O_{12}$), detailing its chemical formula, space group, and a simplified step-by-step synthesis procedure using the solid-state reaction method.

Figure 3 demonstrates MatterChat's advanced reasoning capabilities, showing how it leverages the comprehensive knowledge base of LLMs to address complex materials science challenges. By using a multi-modal query system, MatterChat effectively combines material structure data with textual reasoning. This integration facilitates a working memory scheme [33], which enables the model to provide domain-specific reasoning, detailed synthesis procedures, and explanations that are deeply grounded in the structural properties of materials. Panel (a) presents the chat log for silicon with the space group of i43m. MatterChat not only retrieves the chemical formula and correct space group, but it also provides a rationale for the structural instability of this silicon phase. The model explains that the i43m space group exhibits higher energy per unit cell compared to the thermodynamically stable cubic diamond structure of silicon, making it less likely to occur under standard conditions. Panel (b) illustrates an interaction regarding a popular semiconductor material Gallium Nitride (GaN). Here, MatterChat accurately identifies the chemical formula and space group (P63mc) and constructs a detailed synthesis procedure that aligns with established methods such as molecular beam epitaxy (MBE), metal-organic chemical vapor deposition (MOCVD), and hydride vapor phase epitaxy (HVPE), demonstrating the model's ability to apply structural and contextual knowledge in generating practical scientific outputs. Figure 3(c) explores an interaction for a widely used ferrite material, Yttrium Iron Garnet (YIG, $Y_3Fe_5O_{12}$). MatterChat is able to take the structure and generate detailed text description. Additionally, MatterChat can further generate the synthesis protocol from the preparation of initial materials, their precise mixing ratios, the required sintering conditions, and subsequent characterization techniques, such as X-ray diffraction (XRD) and scanning electron microscopy (SEM). This example demonstrates MatterChat's capability to synthesize and apply domain-specific knowledge effectively, aligning closely with established scientific practice [34].
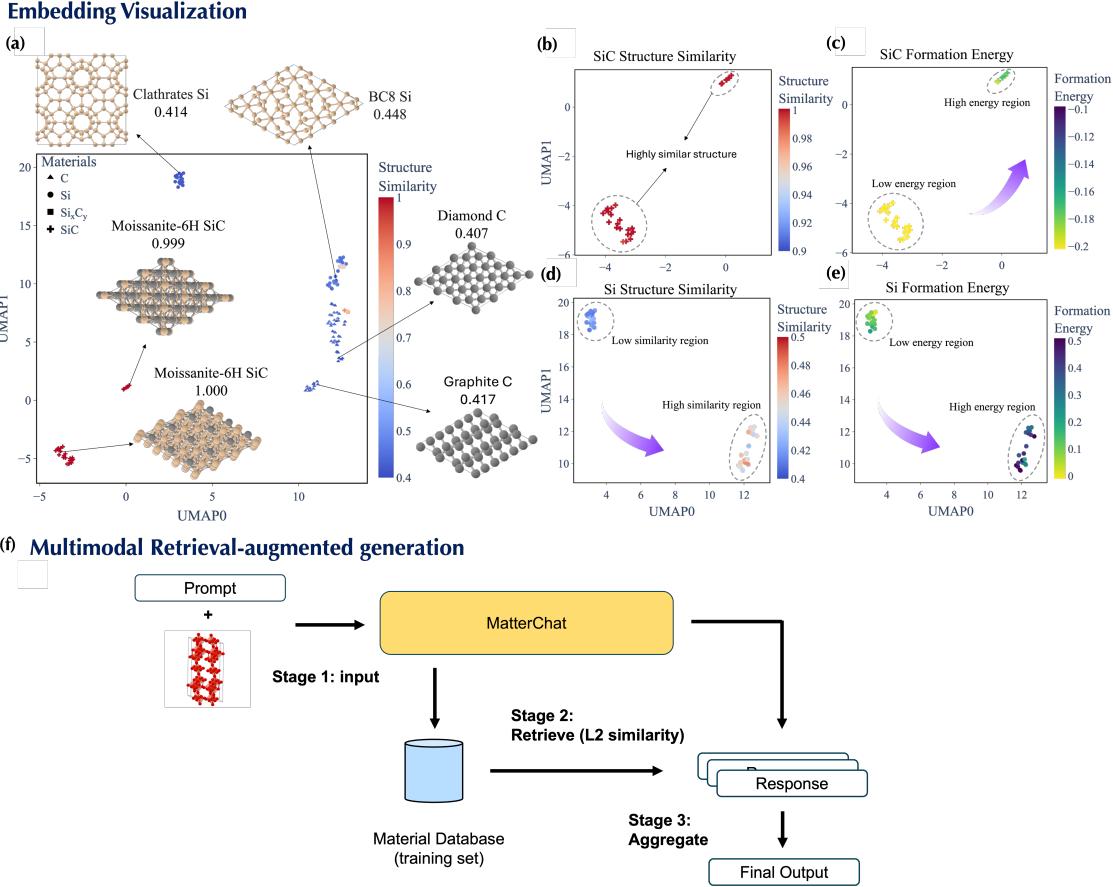
Fig. 4 UMAP visualization of structural embeddings extracted from the bridge model. (a) Visualization of samples containing Si and C elements from the Material Project dataset, showing how materials cluster based on their structural embeddings extracted from the bridge model. (b) Visualization with color-coded structure similarity scores, ranging from low (blue) to high (red), illustrating how materials with similar structures cluster closely together. (c) Visualizations of specific clusters from the embedding space, highlighted to show how the structure similarity metric aids in retrieving materials with comparable structures. (d) Plots with formation energy color coding, demonstrating that structurally similar clusters also correspond to comparable formation energy values, supporting the framework's ability to retrieve relevant candidates with similar properties. (f) Proposed Multi-modal Retrieval-Augmented Generation (RAG) for robust prediction.

2.3 MatterChat extracted embeddings contain structural and property information

We further explore MatterChat's ability to leverage material structural information by providing a detailed visualization/clustering analysis with the UAMP dimension reduction technique [35]. Figure 4(a) to (e) show comprehensive visualizations of embeddings processed by the bridge model, with all material samples that contain silicon (Si), carbon (C), and their composites compounds (e.g., SiC, Si_xC_y) from the Material Project database [36]. UMAP was used to reduce the embeddings from an original 4096 dimensions to two dimensions, with the x and y axes corresponding to the first and second reduced dimensions, respectively.

Figure 4(a) presents the visualizations containing all the selected materials; each sample is color-coded with a structure similarity score [37]. The clustering generally follows distinctions in chemical compositions. Additionally, materials with the same atomic composition are grouped into separate clusters based on crystalline structural differences (e.g., Carbon with Diamond vs Graphite crystalline structure). Figures 4(b) and 4(d) show the filtered visualization/clustering result for materials have single composition of Si and SiC. Figure 4(b) shows the gradient of structure similarity scores, ranging from blue (low similarity) to red (high similarity), demonstrating how closely related structural features result in spatial proximity within the embedding space. However, an interesting exception is observed with SiC: despite its identical composition and similar structural phases, two distinct clusters of SiC emerge, suggesting

that factors beyond composition and structure alone influence their separation. To further explore factors that influence clustering, we labeled the samples according to their formation energy, with results displayed in Figures 4(c) for SiC and 4(e) for Si. These figures clearly show a trend from low to high formation energy. This analysis reveals that clusters grouped by structural similarity also align closely in terms of formation energy. Such findings indicate that the model's ability to produce embeddings that not only differentiate structural characteristics but also correlate with key material properties. Given that the embeddings derived from bridge model preserve both material structure and property-relevant information, we implemented a multi-modal Retrieval-Augmented Generation (RAG) mechanism during inference, as illustrated in Figure 4(f). Instead of relying solely on a single output from MatterChat for each query-sample pair, we now retrieve additional information of two more samples from the material pool (training set). This retrieval is based on the L2 similarity between the embeddings of the sample material and those in the pool. After that we aggregate all three result to get the final output by applying a majority-voting strategy for classification tasks and averaging for quantitative tasks. Such method could further enhance the overall robustness of MatterChat across different tasks. The details of visualization method are provided in Method Section.

2.4 Comprehensive quantitative analysis for all material tasks

To provide a more thorough evaluation of MatterChat, we conducted a comprehensive analysis of its performance across nine material property tasks on the evaluation set (14290 samples). This analysis compares MatterChat to two open-source large language models: (LLMs)—Vicuna [38], and Mistral [17], two physical ML models: SchNet [39] and CHGNet [27]. **Classification Tasks (Figure 5(a)–(f))** Six of the nine tasks are classification tasks, evaluated using prediction accuracy as the metric. These tasks include metallicity, bandgap type, stability, magnetic properties, and experimental observables. As shown in the top two rows of Figure 5, MatterChat demonstrates improvements over all tested models. Compared to state-of-the-art LLMs, MatterChat achieves substantially higher accuracy, benefiting from its ability to integrate graph-based material structure data with natural language reasoning. Moreover, MatterChat even outperforms physical ML models such as SchNet and CHGNet, showing its superior capability in handling multi-modal inputs for material classification.

Numerical Property Prediction (Figure 5(g)–(i)) The remaining three tasks—formation energy, energy above the hull, and bandgap prediction—are numerical property prediction tasks. For these tasks, the mean squared error (MSE) between predicted values and ground truth is used as the evaluation metric. Due to the inherent limitations of LLMs in producing accurate numerical predictions [40], their performance is not included in the bar plots, as the errors were excessively large. Instead, Figure 5 compares MatterChat with the physical ML models. The results show that MatterChat achieves an overall lower RMSE error in the numerical property tasks, outperforming both SchNet and CHGNet. This demonstrates MatterChat's ability to handle highly quantitative material property predictions with precision, further validating the effectiveness of its multi-modal integration approach. Such analysis demonstrates MatterChat's versatility and robustness across diverse material property tasks. By outperforming both state-of-the-art LLMs and physical ML models, MatterChat establishes itself as a powerful tool for materials science applications, offering accurate predictions for both classification and numerical property tasks. These results demonstrate the framework's potential to accelerate material discovery and deepen our understanding of material properties.

2.5 Comparative Study

We performed a comparative study with two popular approaches for training the multi-modal LLMs. 1. Simple Adapter with LoRA finetuning [41]; in this approach, one finetunes the language model using parameter-efficient adapters. 2. Bootstrapping Approach [28]; in this approach, only the bridge model is trained while keeping the graph encoder and LLM frozen, which is the method adopted in our work. Both approaches were evaluated on the same dataset after being trained on identical training sets for the same duration. The results are presented in Table 1. While the Simple Adapter with LoRA finetuning showed improvements over the LLM-only baseline, its performance still lags behind our bootstrapping approach. This suggests that the bootstrapping method is more efficient for this specific problem setup, where the goal is to align material structural data with language representations without extensive finetuning of the underlying models.
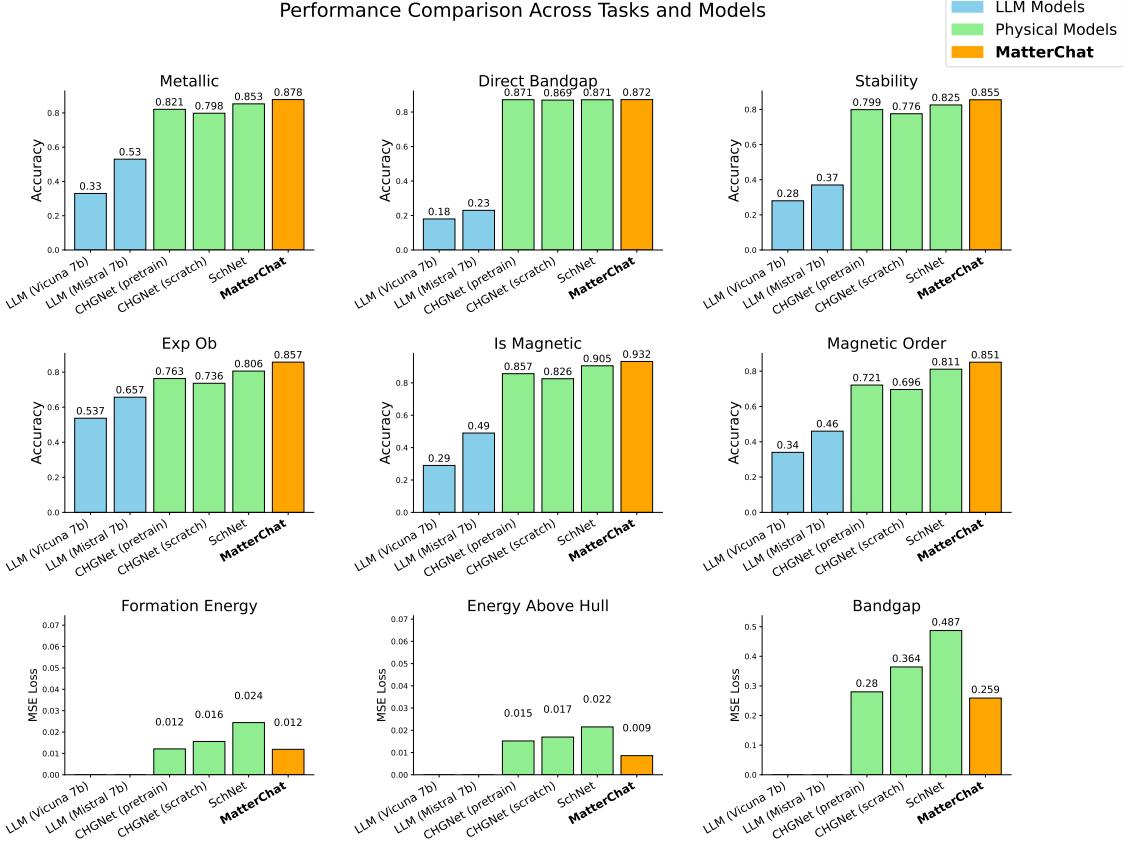
Fig. 5 Performance comparison of MatterChat, open-source LLMs (Vicuna, Mistral), and physical pretrained models (SchNet, CHGNet) across nine material property tasks. (a)–(f) show classification task accuracies, where MatterChat consistently outperforms other models. Panels (g)–(i) present root mean absolute error (RMSE) results for numerical property predictions, demonstrating MatterChat's superior precision in formation energy, energy above the hull, and bandgap tasks.

3 Discussion

In this study, we present MatterChat, a multi-modal framework that demonstrates superior performance in material property prediction and scientific reasoning tasks compared to traditional models. This performance can be attributed to its ability to integrate structural material data with language-based information, creating a more comprehensive representation of materials. Traditional approaches often rely on text-based representations, such as Crystallographic Information Files (.cif), to encode atomic structures. While .cif files effectively capture detailed structural information, their static format may limit the model's capacity to learn complex structure-property relationships when used directly as input. In contrast, MatterChat's multi-modal approach processes structural embeddings derived from atomic graphs

Table 1 Performance comparison with different multi-modal framework structure

Task	Simple Adapter w/ LoRA Finetune LLM	**MatterChat**
Metallic(Accuracy)	0.58	**0.867**
Direct Bandgap(Accuracy)	0.84	**0.8702**
Stability(Accuracy)	0.741	**0.8369**
Exp Ob(Accuracy)	0.715	**0.8119**
Is Magnetic(Accuracy)	0.835	**0.9343**
Magnetic Order(Accuracy)	0.777	**0.8477**
Formation Energy(RMSE)	0.212	**0.1526**
Energy Above Hull(RMSE)	0.1786	**0.1095**
Bandgap(RMSE)	1.52	**0.5428**

Table 2 Material property prediction task results with RAG

Task	MatterChat	MatterChat w RAG
Metallic(Accuracy)	0.867	**0.878**
Direct Bandgap(Accuracy)	0.8702	**0.872**
Stability(Accuracy)	0.8369	**0.855**
Exp Ob(Accuracy)	0.8119	**0.857**
Is Magnetic(Accuracy)	**0.9343**	0.9322
Magnetic Order(Accuracy)	0.8477	**0.8507**
Formation Energy(RMSE)	0.1526	0.1225
Energy Above Hull(RMSE)	0.1095	**0.0949**
Bandgap(RMSE)	0.5428	**0.5070**

alongside textual data, enabling dynamic interactions between atomic configurations and contextual scientific knowledge. This integration enhances the model's generalization ability across diverse material tasks, as evidenced by its improved accuracy in classification and numerical property prediction tasks.

While MatterChat demonstrates advancements in material property prediction and analysis, several limitations provide avenues for future improvement and exploration.
1. Alignment Limitation: One key limitation lies in the current level of alignment between the graph-based material(atom) embeddings and the language representations. Although the framework achieves superior performance on trained material property tasks, this behavior-based alignment does not necessarily imply full representation alignment between the two modalities. Representation level alignment remains an area requiring further investigation [42].
2. Data Limitations: The curated dataset used in this study, while effective for benchmarking, has certain constraints that may impact model generalization ablility. Specifically, the text data for material property tasks consists of a fixed number of paraphrased queries, which could limit the diversity of the language representations. Expanding the dataset to include more comprehensive and diverse textual description scheme, as well as incorporating a broader range of material properties, could address this issue.
3. Frozen LLM: Using frozen LLMs may limit the framework's effectiveness in material-related tasks, as they are primarily trained on broad, general-purpose text rather than domain-specific material science literature. Incorporating specialized LLMs trained on material science datasets could potentially enhance performance by improving domain-specific contextual understanding and reasoning.

To address these limitations, future work could focus on:
1. Improving Alignment: Leveraging advanced techniques to improve representation-level alignment between modalities during end-to-end instructive fine-tuning, such as incorporating contrastive loss at the fine-tuning stage in addition to pretraining to further reinforce structural-textual consistency.
2. Dataset Expansion: Building a more comprehensive dataset with diverse textual queries and a broader range of material properties to ensure the framework's applicability to real-world scenarios.
3. Material Generation Capabilities: Developing a graph generative module to enable the framework to tackle new material design and discovery tasks.
4. Optimizing LLM Integration: Investigating finetuning strategies for LLMs, such as whether multi-modal LoRA finetuning offers advantages over independent LLM finetuning before integration, to improve downstream task performance.

4 Method

4.1 Dataset curation

In this work, we curated a comprehensive dataset from the Materials Project Trajectory (MPtrj) dataset [36], focusing specifically on relaxed samples. By selecting these stable configurations, rather than complete trajectory data, we ensure that the dataset captures the equilibrium states of materials, which are more relevant for downstream tasks such as material property prediction. The final dataset consists of 142,899 high-quality samples, offering a rich and diverse representation of inorganic materials.

To facilitate effective model training and evaluation, we partitioned the dataset into training and testing subsets using a 9:1 split ratio. This ensures that a substantial portion of the data is available for learning, while maintaining a dedicated portion for rigorous performance validation, allowing us to assess the generalization capabilities of the model.

In addition to the relaxed structural data, we retrieved detailed material property information using the Materials Project API [29]. Each material is retrieved by a unique mp-id and is enriched with a variety of key descriptors that span both structural and electronic properties. These include:

- **Structure**: The full atomic structure of the material, detailing atomic positions and bonding.

- **Chemical formula**: The overall chemical composition.

- **Space group**: The crystallographic space group of the material, reflecting its symmetry properties.

- **Crystal system**: The broader classification of the material's crystal structure.

- **Metallicity**: An indicator of whether the material is metallic or insulating.

- **Magnetic properties**: Including whether the material is magnetic and its magnetic ordering (e.g., ferromagnetic, antiferromagnetic).

- **Experimental observables**: Properties that can be compared directly with experimental data.

- **Direct bandgap**: The direct bandgap energy, a key property for semiconductors.

- **Stability**: Indicating whether the material is thermodynamically stable.

- **Energy above hull**: A measure of how stable the material is compared to other phases.

- **Bandgap**: The electronic bandgap, an important factor in determining a material's electronic properties.

- **Formation energy**: The energy required to form the material from its constituent elements.

These attributes offer a comprehensive view of each material, encompassing both its structural arrangement and electronic behavior. By integrating this wealth of data, our model is capable of capturing complex material-property relationships, supporting tasks such as bandgap prediction, stability analysis, and metallicity determination. This dataset not only provides a robust foundation for training ML models, but it also contributes to broader efforts in materials discovery and property optimization.

4.2 Training Detail

MatterChat employs a bootstrapping strategy commonly used in multi-modal learning for vision-language tasks, adapted here for material science applications. The training process consists of two main stages: pretraining to align material structures with descriptive text; and finetuning for both descriptive and property prediction tasks with the LLM module integrated (see Figure S2 in the Supplementary Material). The pretraining phase aims to establish a foundational alignment between material structures and descriptive text. In this stage, the model connects a frozen graph encoder with pairs of graph data and corresponding textual descriptions, without attaching the LLM module. Here, the bridge model acts as a text generator, learning to extract descriptive graph representations that effectively capture structural information relevant to the text data.

This stage consists of three core optimizing targets, each with distinct interaction mechanisms between graph embeddings and text, while maintaining a consistent input format:

1. **Graph-Text Correlation Learning (Contrastive Loss).**
   This task aligns graph and text representations by maximizing the similarity between matched graph-text pairs and minimizing it for mismatched pairs. A contrastive loss is employed:

$$\mathcal{L}_{\text{correlation}} = -\sum_{i=1}^{N} \log \frac{\exp(\text{sim}(q_i, t_i)/\tau)}{\sum_{j=1}^{N} \exp(\text{sim}(q_i, t_j)/\tau)}, \tag{1}$$

   where q_i and t_i represent the graph and text embeddings, respectively, and τ is the temperature parameter controlling the distribution's sharpness.

2. **Graph-Driven Text Prediction (Conditional Language Modeling Loss).**
   The bridge model generates descriptive text based on graph data, conditioned through attention

mechanisms. The loss function is defined as:

$$\mathcal{L}_{\text{prediction}} = -\sum_{t=1}^{T} \log P(y_t | y_{<t}, Q), \tag{2}$$

where Q represents graph query features, and y_t is the token at position t in the output sequence.

3. **Graph-Text Association (Binary Cross-Entropy Loss).**
   This task predicts whether each graph-text pair is correctly matched. A binary cross-entropy loss with hard negative sampling is applied:

$$\mathcal{L}_{\text{association}} = -\sum_{i=1}^{N} (y_i \log(s_i) + (1 - y_i) \log(1 - s_i)), \tag{3}$$

where s_i is the model's prediction score, and y_i indicates whether the pair is matched (1) or not (0).

The total pretraining loss is the sum of the individual task losses:

$$\mathcal{L}_{\text{total}} = \mathcal{L}_{\text{correlation}} + \mathcal{L}_{\text{prediction}} + \mathcal{L}_{\text{association}}. \tag{4}$$

After pretraining, the model undergoes instructive finetuning to optimize its performance on both descriptive and property prediction tasks. In this stage, the pretrained bridge model is integrated with the LLM to enhance multi-modal learning. A fully connected layer is introduced between the bridge model's output and the LLM's input. The finetuning phase includes 12 multi-modal subtasks, including 3 material description tasks and 9 property prediction tasks. Description tasks refine the model's ability to link structural features with detailed textual explanations, while property prediction tasks focus on improving quantitative accuracy in material property estimation. Finetuning is guided by a supervised cross-entropy loss defined as:

$$\mathcal{L}_{\text{finetune}} = -\sum_{i=1}^{N} \sum_{j=1}^{T} y_{i,j} \log P(y_{i,j} | x_i), \tag{5}$$

where $y_{i,j}$ represents the ground truth token for the j-th position of the i-th sample, and $P(y_{i,j} | x_i)$ is the model's predicted probability of the correct token given the multi-modal input x_i.

In the pretraining stage, the model is trained using the AdamW optimizer with a learning rate of 2×10^{-4}, with cosine decay scheduler and linear warmup starting from 1×10^{-6}. A weight decay of 0.05 is applied to regularize the model, with a batch size of 32 and gradient accumulation over 5 steps to manage computational efficiency. Mixed-precision training is enabled to improve performance and reduce memory usage. The model is trained for ~ 25 epochs, with checkpoints saved every 2000 iterations. During the finetuning stage, the AdamW optimizer is again used with a learning rate of 2×10^{-4}, featuring a warmup phase to 1×10^{-4} followed by decay to 1×10^{-5}. The batch size is set to 8, with gradient accumulation over 16 batches to effectively increase the batch size. Finetuning runs for 50 epochs, with checkpoints saved every 300 steps and at the end of each epoch. Additionally, distributed training is implemented using 4 GPUs per node across 8 nodes, leveraging the Distributed Data Parallel (DDP) strategy to enhance training efficiency and scalability.

4.3 Embedding Visualization

The visualization leverages UMAP to reveal chemical insights encoded in the material embeddings that are extracted from the bridge model in a lower-dimensional space. To prepare the data, each high-dimensional embedding, originally structured as (32, 4096), is first flattened into a single vector, capturing the essential features of the material. UMAP is then applied to this set of vectors with number of components equals 2, reducing the data to two dimensions to enable visual interpretation, with random state is set to 1 to ensure consistency in the layout across runs.

Structural similarity scores are computed using the Smooth Overlap of Atomic Positions (SOAP) descriptor [43], combined with the Regularized Entropy Match Kernel (REMatch) [44, 45] to capture the structural characteristics within material embeddings. SOAP is a local atomic environment descriptor that encodes atomic geometries by expanding a Gaussian-smeared atomic density locally, using orthonormal functions derived from spherical harmonics and radial basis functions. From local descriptors to

structure matching, we use REMatch kernel on top of SOAP descriptor. The REMatch kernel considers the best matching of local environments and employs an averaging strategy to enhance structural comparison. For SOAP construction, we consider periodic boundary conditions. The cutoff radius for the local region (r_{cut}), the number of radial basis functions (n_{max}), and the maximum degree of spherical harmonics (l_{max}) are set to 6 Å, 8 Å, and 6 Å, respectively. For the REMatch kernel, the entropic penalty (α) is set to 1, and the convergence threshold is set to (1×10^{-6}). A linear pairwise metric is used for the local similarity calculation.

Acknowledgements

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Supplementary Information:A Multimodal Framework for Material Discovery: Infusing Large Language Models with Atomic Structures

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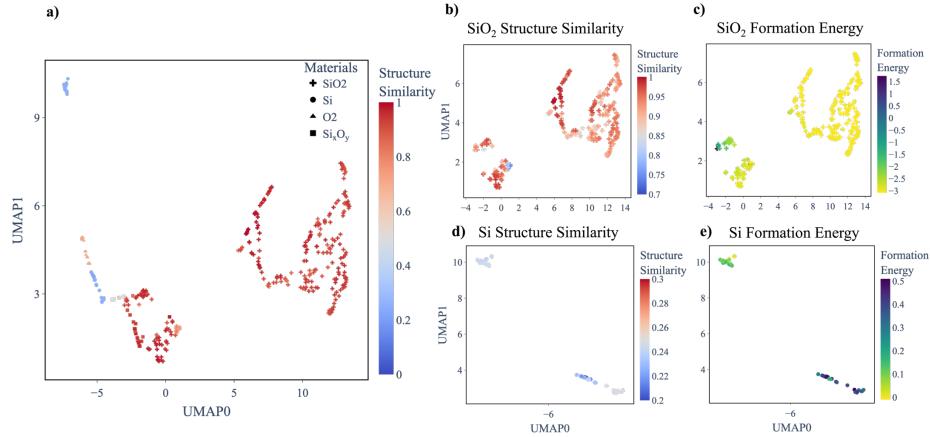
Fig. 1 UMAP visualization of structural embeddings extracted from the bridge model. (Si, O, Si_xO_y)

2

Fig. 2 Training Scheme.

Instruction Templates (descriptive tasks)

Task	Instruction Template
Reduced Formula	<material structure>What is the chemical formula for this material?
	<material structure>Can you tell me the chemical formula of this material?
	<material structure>Please provide the chemical formula for the material.
	<material structure>What is the formula for this material?
	<material structure>Could you tell me the formula of the material?
	<material structure>What elements make up this material?
	<material structure>How would you write the chemical formula of this material?
	<material structure>What is the exact chemical formula of this material?
	<material structure>Can you provide the chemical formula for this material?
Space Group	<material structure>What is the space group for this material?
	<material structure>To which space group does this material belong?
	<material structure>Can you tell me the space group of this material?
	<material structure>Please provide the space group for the material.
	<material structure>What is the crystallographic space group of this material?
	<material structure>How is the space group of this material classified?
	<material structure>Can you specify the space group for this material?
	<material structure>Could you tell me the space group classification of this material?
	<material structure>Can you provide the space group information for this material?
	<material structure>What is the space group number of this material?
Crystal System	<material structure>What is the crystal system of this material?
	<material structure>Can you tell me the crystal system of this material?
	<material structure>Please provide the crystal system for the material.
	<material structure>What crystal system does this material belong to?
	<material structure>How is the crystal system of this material classified?
	<material structure>Can you specify the crystal system for this material?
	<material structure>What is the crystallographic system of this material?
	<material structure>Could you tell me the crystal system classification of this material?
	<material structure>Which crystallographic system does this material belong to?
Generate	<material structure>Can you provide another material similar to this material?
	<material structure>Is there another material like this material that you can provide?
	<material structure>Can you show me a different material similar to this one?
	<material structure>Can you generate another material similar to this one?
General	<material structure>Can you describe this material?
	<material structure><s>

Answer Templates (descriptive tasks)

Task	Instruction Template
Reduced Formula	The chemical formula for this material is <material attribute >.
	The chemical formula of this material is <material attribute >.
	The chemical formula for the material is <material attribute >.
	The formula for this material is <material attribute >.
	The formula of the material is <material attribute >.
	The elements that make up this material are represented as <material attribute >.
	The chemical formula of this material is written as <material attribute >.
	The exact chemical formula of this material is <material attribute >.
	The chemical formula for this material is <material attribute >.
Space Group	The space group for this material is <material attribute >.
	This material belongs to the space group <material attribute >.
	The space group of this material is <material attribute >.
	The space group for the material is <material attribute >.
	The crystallographic space group of this material is <material attribute >.
	The space group of this material is classified as <material attribute >.
	The space group for this material is specified as <material attribute >.
	The space group classification of this material is <material attribute >.
	The space group information for this material is <material attribute >.
	The space group number of this material is <material attribute >.
Crystal System	The crystal system of this material is <material attribute >.
	The crystal system of this material is <material attribute >.
	The crystal system for the material is <material attribute >.
	This material belongs to the <material attribute >crystal system.
	The crystal system of this material is classified as <material attribute >.
	The crystal system for this material is specified as <material attribute >.
	The crystallographic system of this material is <material attribute >.
	The crystal system classification of this material is <material attribute >.
	This material belongs to the <material attribute >crystallographic system.

Instruction Templates (property part1)

Task	Instruction Template
Is Metal	\<material structure>Is this material metal or non-metal?
	\<material structure>Can you tell me if this material is metal or not?
	\<material structure>What is the classification of this material: metal or non-metal?
	\<material structure>Is this material considered a metal?
	\<material structure>How is this material categorized: metal or non-metal?
	\<material structure>Could you specify if this material is metal or non-metal?
	\<material structure>Is the material metallic or non-metallic?
	\<material structure>Can you provide the classification of this material: metal or non-metal?
	\<material structure>Is this material identified as a metal or non-metal?
	\<material structure>What type of material is this: metal or non-metal?
Direct Bandgap	\<material structure>Does the material have a direct bandgap or indirect bandgap?
	\<material structure>Is the bandgap of this material direct or indirect?
	\<material structure>Can you tell me if this material has a direct or indirect bandgap?
	\<material structure>What type of bandgap does this material have: direct or indirect?
	\<material structure>Is this material characterized by a direct or indirect bandgap?
	\<material structure>Could you specify if the bandgap of this material is direct or indirect?
	\<material structure>Does this material exhibit a direct or indirect bandgap?
	\<material structure>Is the bandgap in this material direct or indirect?
	\<material structure>How is the bandgap of this material classified: direct or indirect?
	\<material structure>Is this a direct or indirect bandgap material?
Stability	\<material structure>Is this material stable?
	\<material structure>Can you tell me if this material is stable?
	\<material structure>What is the stability of this material?
	\<material structure>Please provide the stability information for this material.
	\<material structure>Is the material stable under standard conditions?
	\<material structure>Is this material thermodynamically stable?
Experimental Observation	\<material structure>Is the material experimentally observed or not?
	\<material structure>Can you tell me if the material is observed in experiments?
Is Magnetic	\<material structure>Is the material magnetic or not?
	\<material structure>Is the material magnetic or non-magnetic?
	\<material structure>Can you tell me if this material is magnetic?
	\<material structure>What is the magnetic nature of this material?
	\<material structure>Is this material classified as magnetic?
	\<material structure>Does this material have magnetic properties?
	\<material structure>Is this a magnetic or non-magnetic material?
Magnetic Order	\<material structure>What is the magnetic order of the material?
	\<material structure>Can you tell me the magnetic order of this material?
	\<material structure>Could you specify the magnetic order of the material?
	\<material structure>What type of magnetic order does this material have?
	\<material structure>Please provide the magnetic ordering of the material.
	\<material structure>What is the magnetic arrangement in this material?
	\<material structure>Could you tell me the type of magnetic order of this material?

Answer Templates (property part1)

Task	Instruction Template
Is Metal	This material is classified as <material attribute >.
	This material is a <material attribute >.
	The classification of this material is <material attribute >.
	This material is considered <material attribute >.
	This material is categorized as <material attribute >.
	This material is specified as <material attribute >.
	This material is <material attribute >.
	The classification of this material is <material attribute >.
	This material is identified as <material attribute >.
	This type of material is <material attribute >.
Direct Bandgap	The material has a <material attribute >bandgap.
	The bandgap of this material is <material attribute >.
	This material has a <material attribute >bandgap.
	This material has a <material attribute >type of bandgap.
	This material is characterized by a <material attribute >bandgap.
	The bandgap of this material is specified as <material attribute >.
	This material exhibits a <material attribute >bandgap.
	The bandgap in this material is <material attribute >.
	The bandgap of this material is classified as <material attribute >.
	This is a <material attribute >bandgap material.
Stability	This material is <material attribute >.
	Yes, this material is <material attribute >.
	The stability of this material is <material attribute >.
	The stability information for this material is <material attribute >.
	This material is <material attribute >under standard conditions.
	This material is <material attribute >.
Experimental Observation	The material is <material attribute >.
	The material is <material attribute >.
Is Magnetic	The material is <material attribute >.
	This material is <material attribute >.
	Yes, this material is <material attribute >.
	The magnetic nature of this material is <material attribute >.
	This material is classified as <material attribute >.
	This material has <material attribute >properties.
	This is a <material attribute >material.
Magnetic Order	The magnetic order of the material is <material attribute >.
	The magnetic order of this material is <material attribute >.
	The magnetic order of the material is specified as <material attribute >.
	This material has a <material attribute >type of magnetic order.
	The magnetic ordering of the material is <material attribute >.
	The magnetic arrangement in this material is <material attribute >.
	The type of magnetic order of this material is <material attribute >.

Instruction Templates (property part2)

Task	Instruction Template
Bandgap	<material structure>What is the bandgap of the material?
	<material structure>Can you tell me the bandgap of this material?
	<material structure>What is the energy bandgap for this material?
	<material structure>Could you specify the bandgap of the material?
	<material structure>Could you tell me the bandgap energy level of this material?
Formation Energy	<material structure>Can you tell me the formation energy of this material?
	<material structure>Please provide the formation energy for the material.
	<material structure>What is the formation energy value for this material?
	<material structure>How much is the formation energy of this material?
	<material structure>Can you specify the formation energy of this material?
Energy Above Hull	<material structure>Can you tell me the energy above hull of this material?
	<material structure>Please provide the energy above hull for the material.
	<material structure>What is the energy above the hull for this material?
	<material structure>How much is the energy above hull for this material?
	<material structure>Can you specify the energy above hull of this material?
	<material structure>Could you tell me the energy above hull of the material?

Answer Templates (property part2)

Task	Instruction Template
Bandgap	The bandgap of the material is <material attribute >.
	The bandgap of this material is <material attribute >.
	The energy bandgap for this material is <material attribute >.
	The bandgap of the material is specified as <material attribute >.
	The bandgap energy level of this material is <material attribute >.
Formation Energy	The formation energy of this material is <material attribute >.
	The formation energy for the material is <material attribute >.
	The formation energy value for this material is <material attribute >.
	The formation energy of this material is <material attribute >.
	The formation energy of this material is specified as <material attribute >.
Energy Above Hull	The energy above hull of this material is <material attribute >.
	The energy above hull for the material is <material attribute >.
	The energy above the hull for this material is <material attribute >.
	The energy above hull for this material is <material attribute >.
	The energy above hull of this material is specified as <material attribute >.
	The energy above hull of the material is <material attribute >.