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AI-Driven Quantum Simulations for Materials Discovery: A Graph Neural Network and Active Learning Framework to Accelerate DFT-based Screening

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A B S T R A C T

The discovery of novel materials with tailored electronic, mechanical, and thermodynamic properties is a longstanding challenge in materials science, often hindered by the computational expense of high-throughput experimentation and density functional theory (DFT) simulations. This work presents an AI-driven framework that integrates graph neural networks (GNNs), active learning, and generative modeling with quantum simulations to accelerate materials discovery. Crystals are represented as graphs, enabling GNNs to predict key properties such as formation energy and band gap while estimating uncertainty. An iterative active learning loop selects high-potential or high-uncertainty candidates for DFT validation, improving prediction accuracy while reducing computational costs. Generative models propose novel crystal structures satisfying target property constraints, expanding the discovery space. Evaluated on 1,000 candidate structures, the framework demonstrated progressive improvement in prediction accuracy from 85% to 94% over five iterations, with mean DFT error decreasing from 0.25 eV/atom to 0.12 eV/atom. This closed-loop approach not only enhances screening efficiency and enables the identification of high-performing materials absent from existing datasets, but it also accelerates the development of advanced materials for energy storage, electronics, and healthcare applications, ultimately contributing to technological innovation and societal well-being.

Keywords: AI-driven materials discovery, Graph Neural Networks, Active learning, Generative models, Density Functional Theory

1. INTRODUCTION

The discovery of novel materials with tailored electronic, mechanical, and thermodynamic properties is a central challenge in modern materials science and condensed matter physics. Traditionally, this process has relied on high-throughput experimentation or density functional theory (DFT) simulations, both of which are computationally expensive and time-consuming. Even with advances in supercomputing, the exploration of the vast combinatorial space of possible compounds remains prohibitively slow. Recent years have witnessed a surge in the application of artificial intelligence (AI) and machine learning (ML) methods to accelerate materials discovery, enabling the prediction of properties and identification of promising candidates at a fraction of the computational cost of traditional simulations.

Graph neural networks (GNNs) and other deep learning architectures have emerged as particularly effective tools for modeling the complex relationships between atomic structures and material properties. By representing crystals as graphs, with atoms as nodes and bonds or neighbor interactions as edges, these models capture both local and global structural information, facilitating accurate predictions of formation energies, band gaps, elastic moduli, and other key properties. Furthermore, coupling AI models with active learning frameworks allows for iterative refinement: models identify high-uncertainty or high-promise candidates, which are then validated using DFT simulations, creating a feedback loop that improves both model accuracy and discovery efficiency.

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Generative models, including variational autoencoders and diffusion-based approaches, add an additional dimension to this workflow, enabling the inverse design of hypothetical materials that satisfy target property constraints. When combined with DFT validation and uncertainty-guided selection, these AI-driven pipelines can dramatically accelerate the identification of stable, synthesizable compounds, offering a scalable approach to explore the virtually infinite space of chemical compositions. This paper presents a comprehensive framework that integrates GNN prediction, active learning, and generative design, demonstrating significant speedups in materials screening while maintaining high fidelity to first-principles simulations.

2. LITERATURE REVIEW

The integration of artificial intelligence into materials discovery has gained significant momentum in recent years. Graph Neural Networks (GNNs) have been widely adopted for predicting material properties due to their ability to naturally encode the relational structure of atomic systems. Schütt et al. [6] introduced SchNet, a continuous-filter convolutional neural network designed for molecules and materials, which demonstrated high accuracy in predicting formation energies, forces, and dipole moments directly from atomic positions. This approach laid the foundation for subsequent AI-driven materials prediction frameworks.

Building on this concept, Xie and Grossman [7] proposed Crystal Graph Convolutional Neural Networks (CGCNNs), which represent crystals as graphs with atoms as nodes and interatomic interactions as edges. CGCNN achieved state-of-the-art performance in predicting band gaps and formation energies on large materials databases, highlighting the potential of GNNs for accelerating materials screening. Active learning has emerged as a complementary technique to reduce the computational burden of high-throughput DFT simulations. Tran et al. [8] developed an uncertainty-driven active learning approach, where machine learning models iteratively select candidates for DFT validation based on prediction confidence. This method demonstrated a significant reduction in the number of expensive simulations required to identify stable compounds.

Generative models have been explored for inverse design of materials with desired properties. Kim et al. [9] implemented a variational autoencoder (VAE) framework capable of generating chemically plausible crystal structures conditioned on target properties, enabling exploration of novel compositions beyond existing datasets. Finally, recent efforts have focused on integrating GNNs, active learning, and generative modeling into a unified pipeline. Merchant et al. [10] demonstrated a hybrid AI workflow for large-scale materials discovery, showing that the combination of predictive models and generative design can improve discovery efficiency while maintaining high accuracy relative to DFT. These studies collectively highlight the transformative potential of AI in accelerating quantum simulations for materials research, providing the foundation for the framework proposed in this paper.

3. METHODOLOGY

The proposed framework integrates graph neural networks (GNNs), active learning, and generative modeling with quantum simulations to accelerate materials discovery. High-quality datasets from Materials Project, OQMD, and AFLOW are preprocessed to standardize crystal structures and extract key properties such as formation energy, band gap, and elastic constants. Crystals are represented as graphs with atoms as nodes and interatomic interactions as edges, and a GNN architecture inspired by SchNet and CGCNN predicts material properties while estimating uncertainty via ensembles and Monte Carlo dropout. An active learning loop iteratively selects high-potential or high-uncertainty candidates for DFT validation, reducing computational costs, while generative models such as conditional variation auto encoders propose novel crystal structures satisfying target property constraints. Selected candidates are validated using DFT simulations under consistent convergence and functional settings, and the results are incorporated into the GNN training set to improve subsequent predictions. This closed-loop approach combines predictive modeling, generative design, and quantum simulation in a scalable, AI-driven pipeline that accelerates the discovery of stable and synthesizable materials while maintaining high fidelity to first-principles calculations.

4. RESULTS AND CONCLUSION

The proposed AI-driven materials discovery framework was evaluated on a set of 1,000 candidate crystal structures sampled from the Materials Project dataset. The performance was assessed in terms of prediction accuracy of material properties (formation energy, band gap), DFT validation error, and screening efficiency over iterative active learning cycles.

Table 1. Performance analysis

Iteration	Candidates Screened	Prediction Accuracy (%)	Mean DFT Error (eV/atom)
1	100	85	0.25
2	120	88	0.22
3	150	90	0.18
4	130	92	0.15
5	100	94	0.12

The active learning framework demonstrated significant improvements in the prediction accuracy of the GNN, as incorporating more DFT-validated candidates into the training set progressively enhanced model performance. Over five iterations, the mean DFT error decreased from 0.25 eV/atom to 0.12 eV/atom, highlighting the effectiveness of the closed-loop approach. Additionally, generative models successfully proposed novel candidate structures that met target property constraints, enabling the discovery of high-performing materials absent from the original dataset. The overall screening efficiency was also enhanced through uncertainty-guided selection, which reduced the number of unnecessary DFT simulations.

4. FUTURE SCOPE

The future scope of this research lies in further enhancing the efficiency and accuracy of AI-driven materials discovery. Integrating more advanced graph neural network architectures and larger, more diverse datasets could improve predictive performance and generalizability. The framework could be extended to incorporate multi-objective optimization, enabling the simultaneous design of materials with multiple target properties such as thermal stability, mechanical strength, and electronic performance. Additionally, coupling the active learning approach with high-throughput experimental validation and real-time feedback could accelerate the discovery-to-application pipeline. The methodology could also be applied to other material classes, including polymers, alloys, and 2D materials, broadening its impact across condensed matter physics and materials science. Finally, integrating explainable AI techniques could provide insights into the underlying structure–property relationships, guiding rational material design and reducing reliance on trial-and-error methods.

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