Accelerated Discovery of Electride Materials Using Generative AI and Hierarchical Screening

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Introduction

- **Electrides** are materials in which electrons occupy interstitial spaces within a crystal lattice rather than remaining bound to individual atoms, promising for superconductors, catalysts, batteries, and advanced electronic devices.
- **Density Functional Theory (DFT)** accurately predicts material properties but is computationally expensive for large-scale materials screening.
- **MatterGen**, a generative AI model, rapidly generates candidate structures,.
- **MatterSim**, a deep-learning framework to relax the structure, reducing the cost for DFT calculations required.
- **This Project** integrates ElectrideFlow, MatterGen, MatterSim, and high-performance computing to accelerate the discovery of novel electride materials.

Objectives

- **AI-generative workflow** to accelerate the discovery of novel electride materials.
- **Fine-tune** the MatterGen generative model on the HPC cluster for crystal structure generation.
- **Generate** candidate crystal structures for screened ternary electride compositions.
- **Evaluate** AI-generated structures using MatterSim prior to computationally intensive DFT calculations.
- **Establish** a scalable workflow for future high-throughput electride discovery.

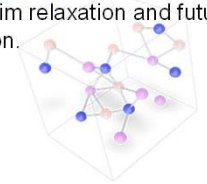
Method

Computational Workflow

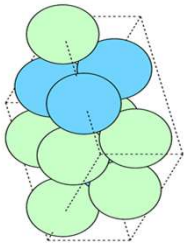
ElectrideFlow 1
(Design Chemical Space)
↓
MatterGen
(Fine-Tune & Generate Structures)
↓
MatterSim
(Relax & Evaluate Structures)
↓
ElectrideFlow 2
(Identify Interstitial Electrons)
↓
Future DFT
(VASP)

Collected Data

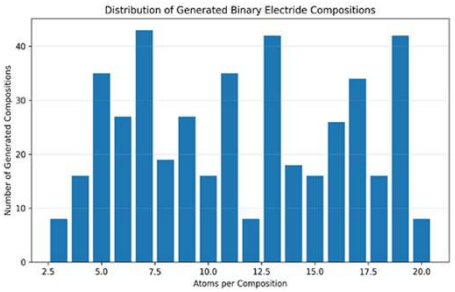
- **146,436** Li-B-N ternary candidate compositions identified using ElectrideFlow.
- **17** crystal structures generated for the test composition $Li_1B_1N_1$ using MatterGen.
- **Structures** generated across six supercell sizes (up to 20 atoms per cell).
- **100%** successful crystal structure generation.
- **AI-generated** structures prepared for MatterSim relaxation and future DFT validation.



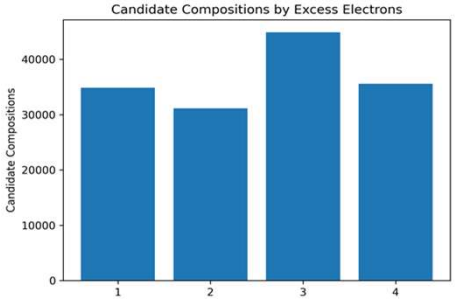
Results



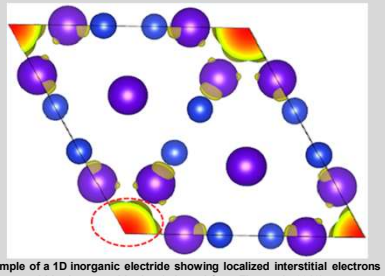
• Optimized $Li_1B_1N_1$ crystal structure after MatterSim BFGS relaxation. The dashed outline indicates the relaxed unit cell.



• Distribution of AI-generated ternary candidate compositions identified during computational screening.



- Distribution of the 146,436 screened ternary candidate compositions grouped by excess electron count



• Example of a 1D inorganic electride showing localized interstitial electrons within the crystal lattice (adapted from Zhu et al., 2018).

Conclusions

- **Successfully** fine-tuned MatterGen on the HPC cluster to generate candidate inorganic crystal structures for electride discovery.
- **Integrated** ElectrideFlow, MatterGen, and MatterSim into an AI-driven workflow for efficient materials screening.
- **Screened** 146,436 ternary candidate compositions and generated representative crystal structures for further evaluation.
- **Established** a scalable framework to accelerate electride discovery and support future DFT (VASP) validation of promising candidates.

References

(1) Zeni, C., Pinsler, R., Zügner, D., et al. (2025). A Generative Model for Inorganic Materials Design. Nature.

(1) Tao, S., & Zhu, Q. (2026). Accelerated Inorganic Electrides Discovery by Generative Models and Hierarchical Screening. arXiv:2601.21077.

(1) Chen, T., et al. (2024). MatterSim: A Deep Learning Potential for Atomistic Materials Simulations. arXiv.

(1) Kresse, G., & Furthmüller, J. (1996). Efficient Iterative Schemes for Ab Initio Total-Energy Calculations Using a Plane-Wave Basis Set. Physical Review B, 54(16), 11169–11186.