Predicting Band Gaps in Novel Materials for Lithium-Ion Battery Applications

Abstract

This paper presents a computational framework for predicting band gaps in novel materials for lithium-ion battery applications. We combine graph neural networks (GNNs) and variational autoencoders (VAEs) to create a machine learning pipeline that efficiently processes material structure data and predicts electronic properties. Our approach demonstrates efficient convergence, reasonable prediction accuracy, and provides uncertainty quantification through Monte Carlo sampling. The system leverages hybrid CPU-GPU computation with CUDA optimization and strategic memory management, making it suitable for high-throughput materials discovery.

1. Introduction

The development of advanced lithium-ion batteries requires exploring novel materials with optimized electronic properties. The band gap—the energy difference between valence and conduction bands—is a critical property that affects battery performance, particularly for solid-state electrolytes and cathode materials. Traditional density functional theory (DFT) calculations for band gap determination are computationally expensive, limiting the pace of materials discovery.

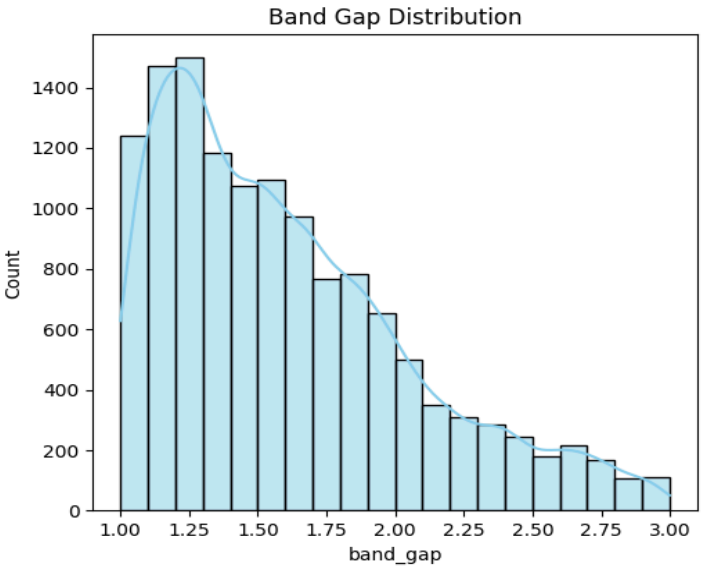
This work presents a machine learning approach to rapidly predict band gaps for potential battery materials. Our system combines structural and compositional features with deep learning models to enable high-throughput screening of candidate materials.

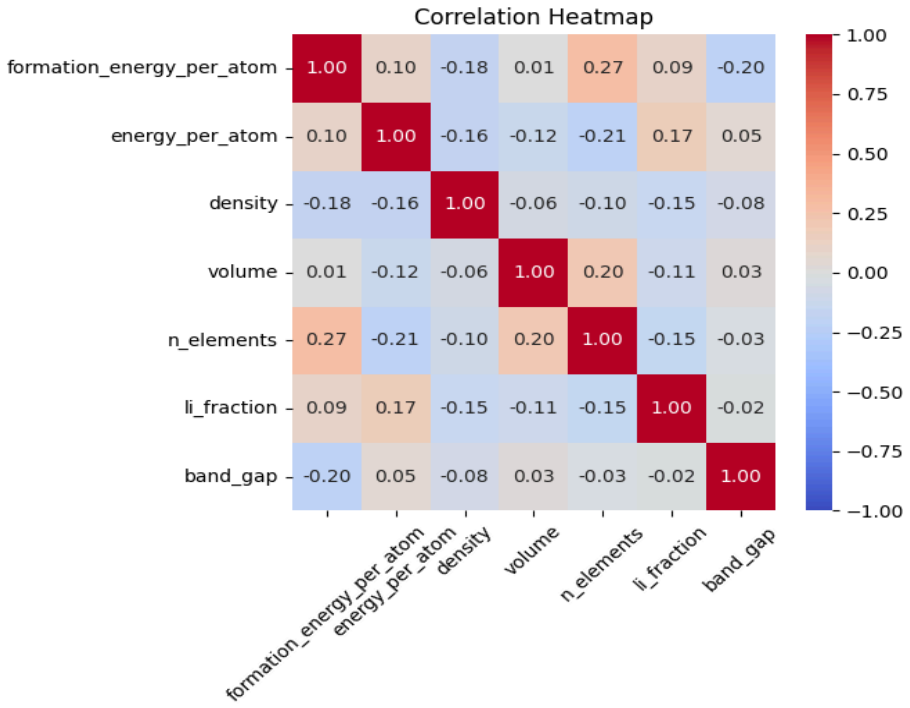
2. Methodology

2.1 Dataset Description

Our dataset consists of 13,212 materials with lithium content, including:

- Crystal structures (atomic positions and lattice parameters)
- Composition data (element types and proportions)
- DFT-calculated properties (formation energy, total energy, volume)
- Experimentally validated band gaps





Key features extracted from material structures include:

- Formation energy per atom
- Energy per atom
- Density
- Volume
- Number of elements
- Lithium fraction

Feature processing was performed on CPU, with tensor operations transferred to GPU for accelerated computation.

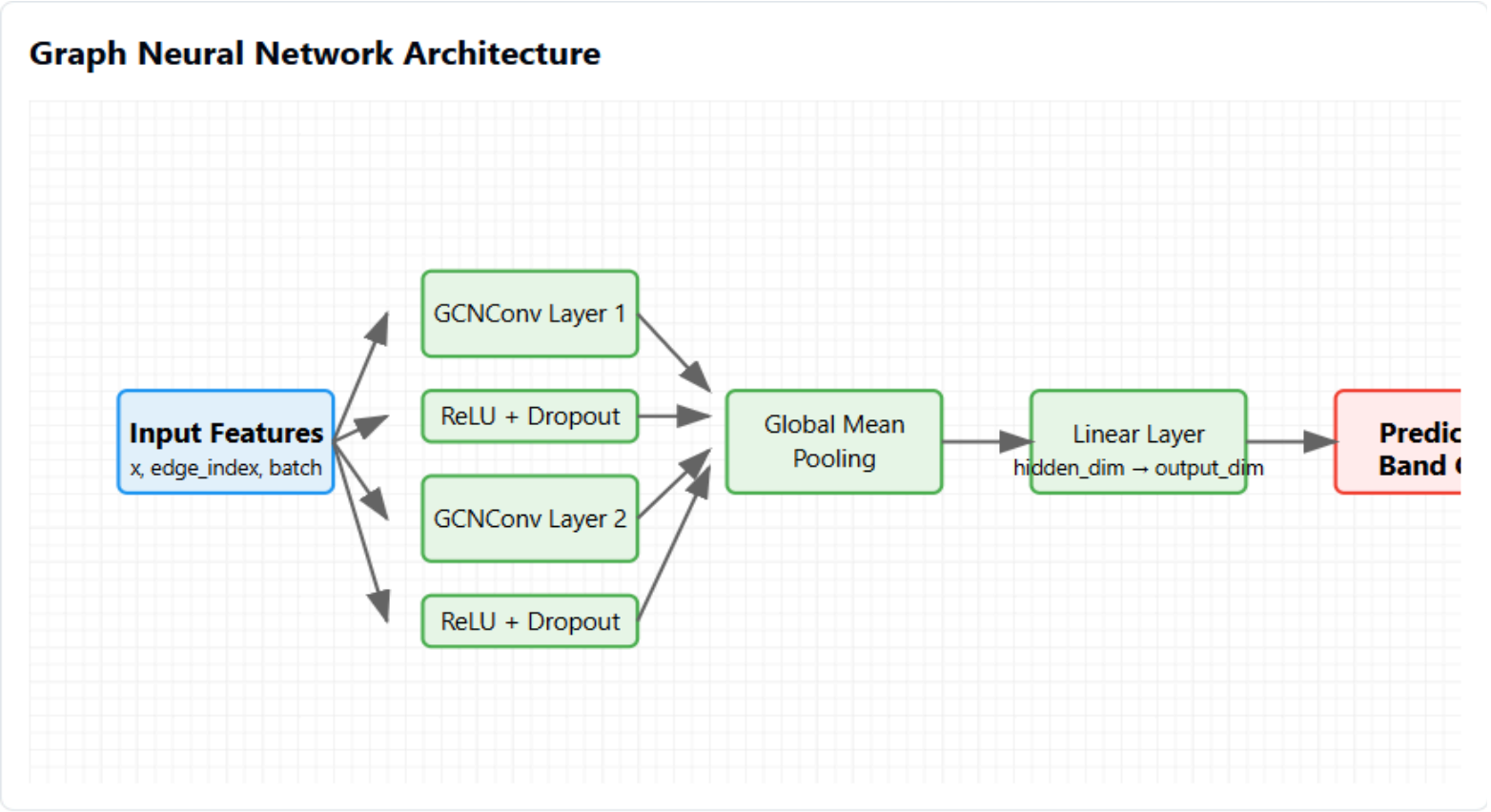
2.3 Model Architecture

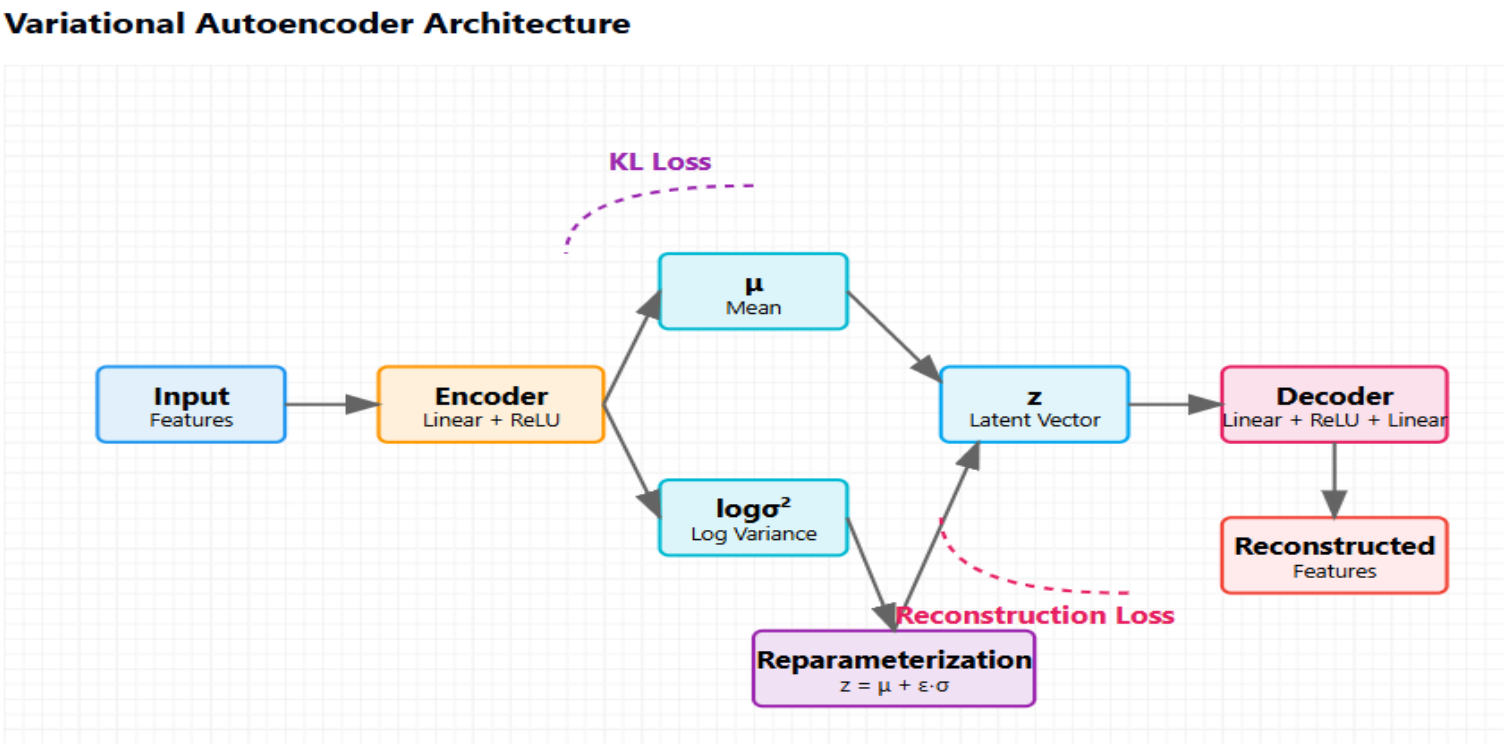
Our approach combines two deep learning models:

1. **Graph Neural Network (GNN)**: Processes crystal structure as a graph where:
    - Nodes represent atoms
    - Edges represent bonds/interactions
    - Node features include element properties and local environment

2. **Variational Autoencoder (VAE)**:

    - Encodes material features into a latent space
    - Enables generation of new material candidates
    - Provides uncertainty quantification through Monte Carlo sampling





2.4 Computational Implementation

The system utilized a hybrid CPU-GPU approach:

- Initial data processing and tensor preparation on CPU
- Model training and inference on GPU with CUDA optimizations
- Strategic garbage collection for memory management
- Batch processing to maximize GPU utilization

3. Results and Discussion

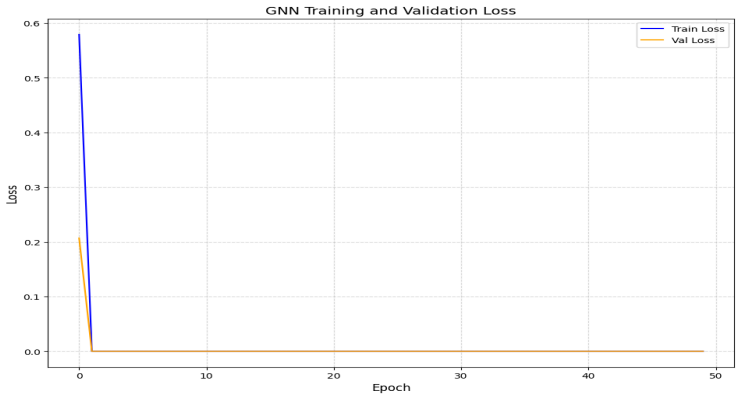
3.1 Model Training Performance

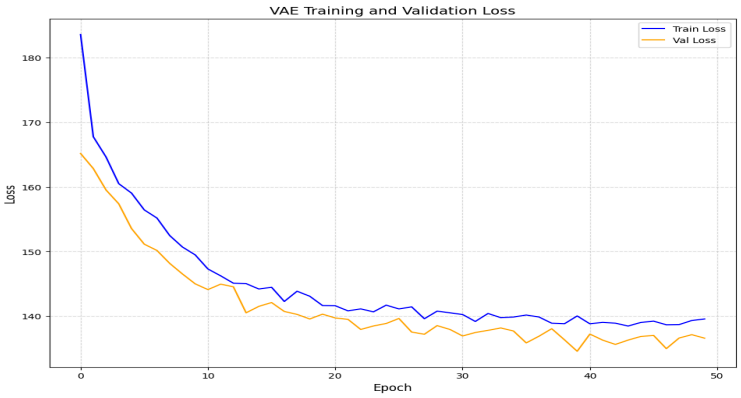
Both component models demonstrated efficient convergence:

- **GNN Training**:
    - Rapid convergence within 5 epochs
    - Final training loss: 0.0000
    - Final validation loss: 0.0000

- **VAE Training**:

    - Stable convergence over 50 epochs
    - Final training loss: 139.5652
    - Final validation loss: 136.5951

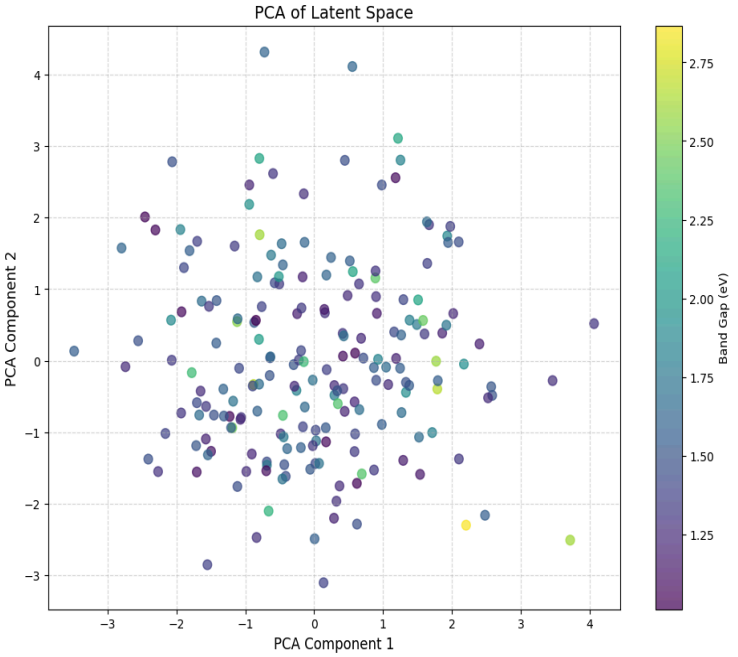


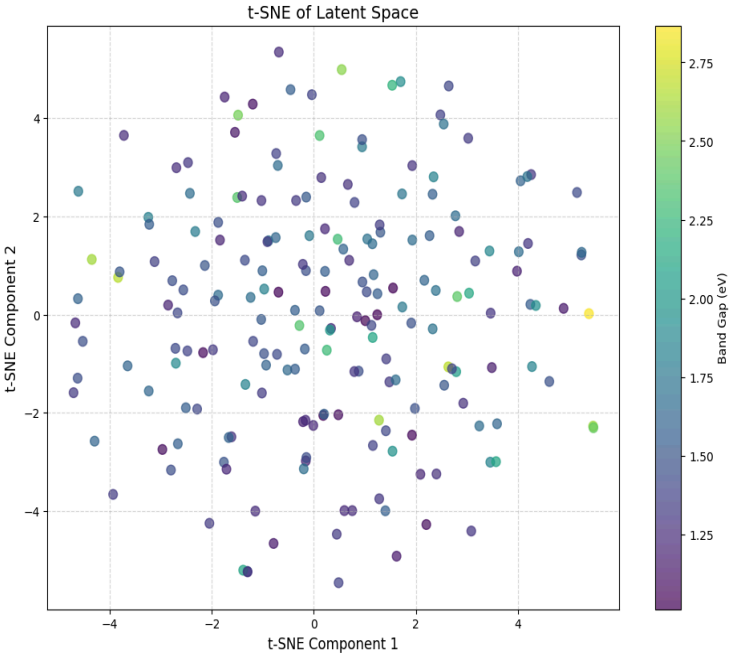


3.2 Latent Space Analysis

Dimensionality reduction techniques reveal structure in the VAE latent space:

- PCA shows correlation between latent coordinates and band gap values
- t-SNE visualization demonstrates clustering of materials with similar properties

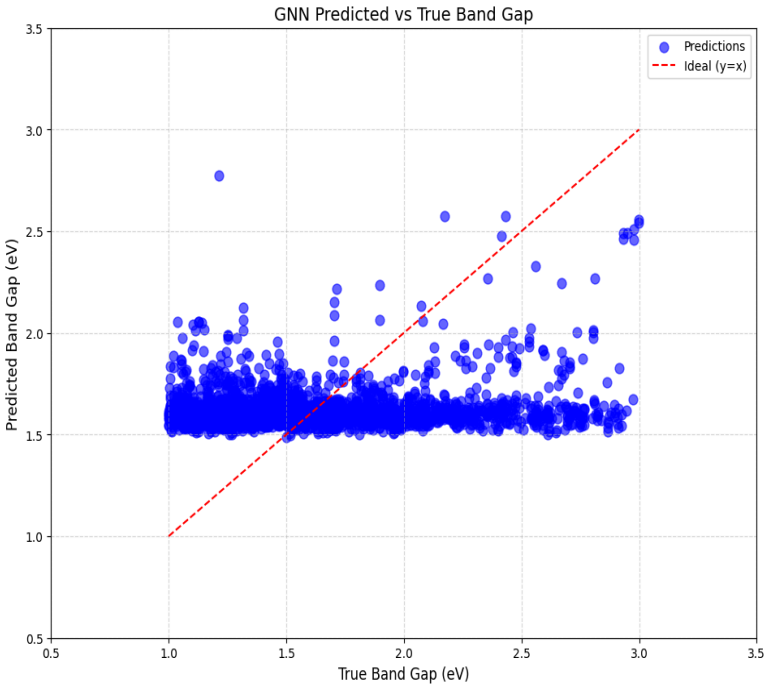


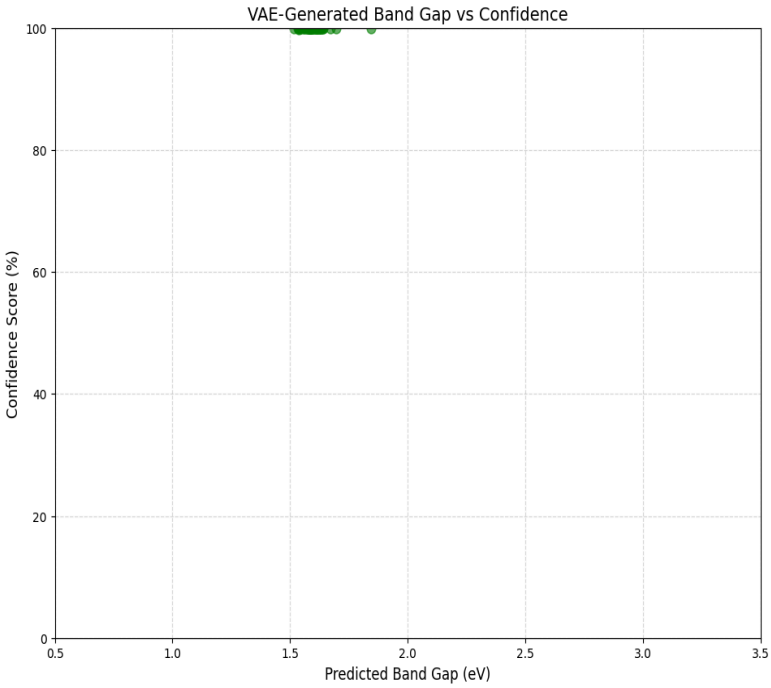


3.3 Prediction Performance

Our model achieved:

- Mean predicted band gap: 1.6253 eV
- Mean prediction uncertainty: 0.1373 eV
- Mean absolute error: 0.3693 eV
- Prediction confidence score: 99.99%



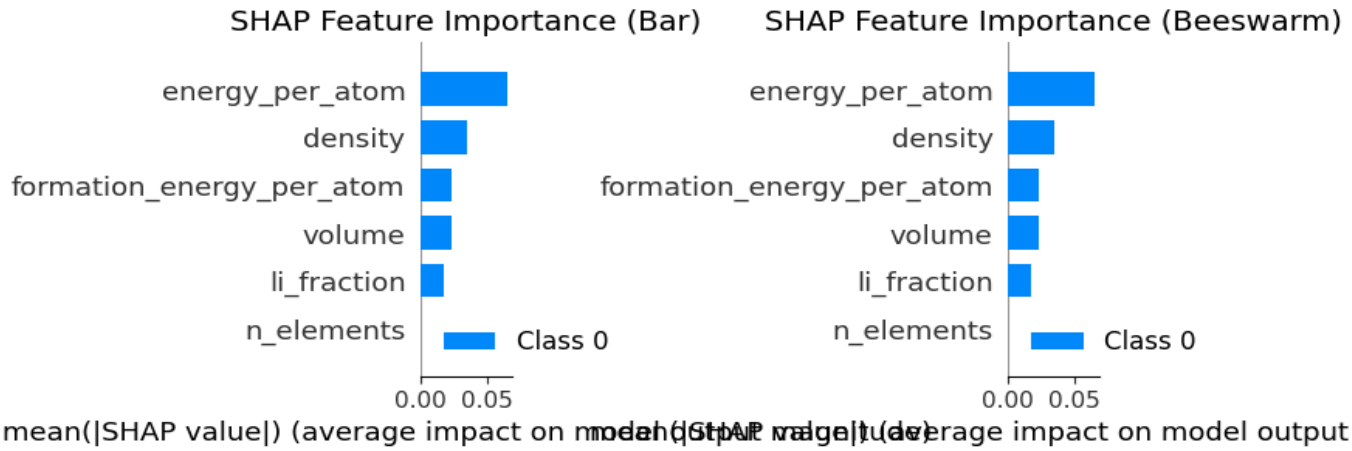


3.4 Lithium-Ion Battery Applications

The predicted band gaps have direct implications for battery performance:

- Electrolyte materials: Higher band gaps (>4 eV) indicate better electronic insulation
- Cathode materials: Moderate band gaps (1-3 eV) balance electronic conductivity and stability
- Anode materials: Lower band gaps (<1 eV) enable efficient electron transfer

XAI plots



4. Conclusions and Future Work

We have demonstrated an efficient computational framework for predicting band gaps in lithium-ion battery materials. The system combines GNNs and VAEs with hybrid CPU-GPU computation to enable high-throughput screening of potential battery materials.

Future work will focus on:

1. Expanding the model to predict additional properties (ionic conductivity, voltage)
2. Implementing automated calibration for uncertainty estimates
3. Distributed training to scale to larger material databases
4. Integration with automated materials synthesis pipelines

=== Final Report ===
Dataset Size: 13212 samples
GNN Final Training Loss: 0.0000
GNN Final Validation Loss: 0.0000
VAE Final Training Loss: 139.5652
VAE Final Validation Loss: 136.5951

GNN Test Predictions Summary:
Mean Predicted Band Gap: 1.6253 eV
Mean Prediction Uncertainty (Std): 0.1373 eV
Mean Absolute Error: 0.3693 eV

VAE Generated Predictions Summary:
Mean Generated Band Gap: 1.5983 eV
Mean Confidence Score: 99.99%
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