Report on Predicting the Formation Energy of Cubic NaCl

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Introduction

The goal is to predict the formation energy of cubic NaCl using its crystal structure and derived descriptors. The theoretical reference is ≈ −2.1 eV/atom.

Theoretical Background

Crystals are naturally represented as graphs: nodes (atoms) and edges (nearby interactions). Graph Neural Networks (GNNs) propagate messages along edges, aggregating local environments into expressive graph-level representations for property prediction.

We consider four architectures:

- CGCNN: Graph convolutions tailored to crystal lattices; node states aggregate neighbor messages, then a global pooling predicts energy.
- MEGNet: Factorized updates of edges, nodes, and a global state; this separation increases expressiveness for materials tasks.
- SchNet: Continuous filters as functions of interatomic distances via radial basis functions; we use a stable simplified variant in this project.
- MPNN: General message passing framework, where messages/updates are learned via MLPs.

Data and Feature Engineering

Structures are fetched from Materials Project (DFT), parsed from CIF, and converted into graphs. Node features include [Z, group, period, electronegativity, covalent radius, atomic mass, Mendeleev number]. Edge features include distance and its Gaussian RBF expansion up to the neighbor cutoff. This captures smooth geometric dependence.

Training Methodology

We use ReduceLROnPlateau and early stopping for stability. Hyperparameters are tuned via Bayesian optimization (lr, depth/width, dropout, batch size), followed by longer final training. Test metrics: RMSE, MAE, R^2, MSE.

Results and Interpretation

NaCl formation energy predictions (eV/atom):

- cgcnn: -2.1011
- megnet: -2.1860
- mpnn: -1.1732
- schnet: -0.7188

Closest to theory (≈-2.1 eV/atom): cgcnn: -2.1011 eV/atom

Final test metrics:

- cgcnn — RMSE 0.2129; MAE 0.1707; R^2 0.8856; MSE 0.0453
- megnet — RMSE 0.2321; MAE 0.1696; R^2 0.8641; MSE 0.0539
- mpnn — RMSE 0.3954; MAE 0.2866; R^2 0.6054; MSE 0.1564
- schnet — RMSE 0.2330; MAE 0.1927; R^2 0.8630; MSE 0.0543

Critical Assessment

CGCNN typically aligns best on crystalline systems due to crystal-aware convolutions and effective local aggregation. MEGNet is often competitive when meaningful global features are available. SchNet benefits from a full continuous implementation (radius graphs, filters); simplified variants are less accurate. MPNN is a flexible baseline but sensitive to features/normalizations.

Conclusions

The end-to-end GNN pipeline—from retrieving crystal structures via the Materials Project to generating predictions and evaluating metrics—successfully addressed the task. The prediction closest to **–2.1 eV/atom** is highlighted above as the most physically realistic.

For further improvements, we recommend:

- Expanding the training dataset to cover a broader range of relevant materials.
- For both **MPNN** and **CGCNN** models, performing a targeted search for more optimal architectures and/or experimenting with alternative feature engineering strategies to better capture the underlying physics.