

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 and validation of the neural networks were performed on a representative set of alkali halides in various crystal structures (excluding the cubic and triclinic forms of NaCl). This set included compounds of the type AX where A $\in \{\text{Li}, \text{Na}, \text{K}, \text{Rb}, \text{Cs}\}$ and X $\in \{\text{F}, \text{Cl}, \text{Br}, \text{I}\}$.

For prediction and the final evaluation of model performance, the cubic (rock-salt) phase of NaCl was held out and used as the target system.

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, R², MSE.

Results and Interpretation

NaCl formation energy predictions (eV/atom):

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

Closest to theory (\approx -2.1 eV/atom): cgcn: -2.1011 eV/atom

Final test metrics:

- cgcn — RMSE 0.2129; MAE 0.1707; R² 0.8856; MSE 0.0453
- megnet — RMSE 0.2321; MAE 0.1696; R² 0.8641; MSE 0.0539
- mpnn — RMSE 0.3954; MAE 0.2866; R² 0.6054; MSE 0.1564
- schnet — RMSE 0.2330; MAE 0.1927; R² 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.