Developing a sequential learning methodology in order to discover novel anti-perovskite and garnet-structured materials

Predictive Science & Engineering Design Project (2019-2020)
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**RESEARCH GOALS**

1. Discovery of new, stable antiperovskite structures
2. Discovery of new, stable garnet structures
3. Development of a scalable, reproducible computational framework that accelerates the discovery of new materials

**METHOD OF RESEARCH**

A sequential learning framework that combines high-throughput density functional theory with machine learning in a cycle of training, predicting, validating and retraining until convergence.

**Tools used**

- Open Quantum Materials Database (OQMD),
- Crystal Graph Convolutional Neural Network (CGCNN),
- Vienna Ab Initio Simulation Package (VASP)

**ANTIPEROVSKITE RESULTS**

- 35 NEW compounds discovered
  - 14 stable
  - 21 metastable

**GARNET RESULTS**

- 153 NEW compounds discovered
  - 110 stable
  - 43 metastable

**Key Takeaways**:

- CGCNN model has low MAE
- CGCNN depends on having structure-type in training set for higher accuracy.
- Multiple rounds of training and predicting are vital
- Multiple models trained on varying amounts of data are vital

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**GARNET RESULTS**

- ML vs DFT Mean absolute error (MAE): 157 meV/atom
- ML success rate of 31% very high (previous HT-study success rate ~10%)
- We recommend 6 compounds to be interesting and worth exploring more computationally and experimentally