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Machine Learning for Materials Study

Machine learning is emerging as a powerful tool to accelerate materials discovery across a wide range of chemical compositions and property spaces. In this work, we apply state-of-the-art machine learning techniques to two classes of functional materials: Heusler alloys and hybrid organic-inorganic perovskites (HOIPs).

Heusler alloys, discovered at the end of the nineteenth century, have emerged as exciting materials in the 21st century due to their fascinating properties, such as half-metallicity, martensitic transformation, and ferromagnetism. These properties make Heusler alloys promising candidates for applications in spintronics and thermoelectric devices. In this study, we aim to discover new Heusler alloys using state-of-the-art machine learning approaches.

Our dataset includes 423 distinct X_2YZ ternary full Heusler compounds, where X and Y are transition metals (from the d-block of the periodic table), and Z is a main-group element. We apply supervised machine learning methods—including Kernel Ridge Regression (KRR), Support Vector Machines (SVMs), Random Forest, and Gaussian Process Regression—to model and predict the formation energy of new Heusler alloys.
Among these models, KRR demonstrates the highest accuracy for our dataset. After validating the model, we use it to predict new Heusler alloys. Our study provides valuable insights that can guide both computational screening and experimental synthesis of novel Heusler materials.

In parallel, we also explored dimensionality prediction in hybrid organic-inorganic perovskites (HOIPs), where dimensionality plays a critical role in determining the material's electronic properties, optical, and stability. Using a curated dataset of experimentally synthesized HOIPs, we extract a set of descriptors as well as add engineered features to improve model accuracy
and generalization. A classification model is trained to predict 0D, 1D, 2D, and 3D structural dimensionality, enabling high-throughput screening of candidate HOIPs. This predictive model facilitates the design of perovskites with targeted dimensionality.

Topical Area

AI and data science

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