Evaluation Framework for Thermodynamic and Chemical Validity in Generative Composition Models

Tomiya Yamamoto
Nara Intitute of Science and Technology

In recent years, materials informatics which leverages artificial intelligence to accelerate materials discovery, has attracted significant attention as a promising approach in materials science.
Among its various techniques, generative models have shown particular promise in the design of novel compounds by learning the underlying distributions of existing datasets.
Recently, these models have begun to be applied to materials design, particularly for the exploration of new chemical compositions.
However, quantitative metrics for assessing the chemical validity of generated novel compositions have yet to be firmly established.
In this study, we propose chemically grounded evaluation metrics based on valence balance and electronegativity balance, enabling more interpretable and consistent assessment of generated compositions.
Additionally, to evaluate the thermodynamic stability of the generated compositions, we tested multiple crystal structure prediction models with energy above hull calculations.
This multi-model strategy helps mitigate biases and errors that may arise from relying on a single structural predictor.
We apply this evaluation framework to the outputs of our previously developed generative model, which is capable of generating compositions that satisfy target material properties.
Our results demonstrate that the proposed framework enables accurate evaluation of both chemical plausibility and thermodynamic consistency of generative outputs.