Designing new materials by closed loop consisting of GAN and first-principles calculation

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Materials development requires a high level of knowledge and creativity. In particular, designing a material that exhibits the desired physical properties is called an inverse problem, and is one of the most difficult problems in materials sciences. The objective of this study is improvement of the efficiency of new material design by using materials data and machine learning to mimic the knowledge and creativity of scientists. In this study, a generation scheme for crystal structures with desired properties is established by combining two models: a generative model based on an adversarial generative network that proposes a chemical composition with desired properties, and a model that predicts a crystal structure from the chemical composition. The generated 83 materials were confirmed by DFT calculations to exhibit the formation energies close to the desired values. In the future, we aim to extend the training data with the generated data to be able to generate more diverse compositions for extrapolated regions.