Inorganic Materials Design Utilizing Machine Learning and Generative Adversarial Networks

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Discovering materials that satisfy target properties poses a fundamental inverse design challenge, which has traditionally depended on expert try-and-error and heuristic knowledge. With the rise of machine learning, data-driven generative approaches are gaining attention as a means to accelerate this process. In our work, we utilize a conditional generative adversarial network (CompGAN) to produce novel chemical compositions conditioned on specified formation energy values. Since these generated compositions typically lack known structural prototypes, we integrate a machine learning-based crystal structure prediction framework (CSPML) to estimate likely crystal structures, which are subsequently validated using first-principles calculations. Our results show that CompGAN is capable of generating candidates with formation energies aligned with target values (e.g., –3.0 eV/atom), supporting its utility in suggesting realistic materials. In addition, we establish a closed-loop workflow that iteratively retrains the generative model with feedback from newly computed data, thereby extending the search into unexplored composition spaces. As part of this study, we are also addressing the challenge of multi-objective optimization for simultaneous control of multiple desired properties, which will be introduced in the presentation.