

Integration of Generative Deep Learning in Metaheuristic Algorithms for Crystal Structure Prediction

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The generation of periodic structures of stable materials is a long-standing, open problem for the material design community. The constraints that define the stability of a material is the root of this problem. One, the global stability of a structure requires specific bonding between element types, and two, atomic coordinates must lie within energy minimas defined by quantum mechanics. Existing methods used to tackle this problem include random searches, metaheuristic algorithms and generative machine learning models, where each method type has its advantages and shortcomings. Data-driven machine learning methods have the potential to expedite the rate of materials design by bypassing bottlenecks found in metaheuristic algorithms used for crystal structure prediction. In this work, we integrate a Wasserstein generative adversarial network into a genetic algorithm for structure prediction (GASP) where synthetic novel materials with targeted characteristics such as low formation energy will be generated through the sampling of the WGAN's latent space and subsequently optimized through the GASP framework, leading to the discovery of novel, stable ground-state structures.