Machine Learning Accelerated Genetic Algorithms for Computational Materials Search

A machine learning (ML) model is trained on-the-fly as a computationally inexpensive energy predictor before analyzing how to augment convergence in Genetic Algorithm (GA)-based approaches by using the ML model as a surrogate. This leads to a machine learning accelerated genetic algorithm (MLaGA) combining robust qualities of the GA with rapid learning of the ML. The MLaGA is used to search for stable, compositionally variant nanoparticle alloys to illustrate its capability for accelerated materials discovery, e.g., nanoalloy catalysts. The MLaGA, in this case, yields a 50-fold reduction in the number of required energy calculations compared to a traditional "brute force" GA. This makes searching through the space of all compositions of a binary alloy particle in a given structure feasible, using density functional theory calculations.