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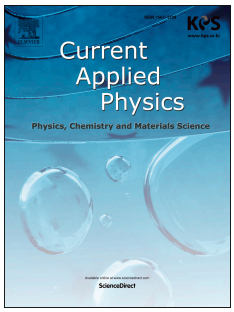

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An improved Genetic Algorithm for Crystal Structure Prediction

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ABSTRACT

We present an improved genetic algorithm (GA) for crystal structural prediction based on empirical potentials with a higher convergence rate. Some of the existed methods for crystal structure prediction *via* GA are much likely to suffer from stagnation during evolution, with a consequent loss of productivity and search depth. Some approaches, which include penalizing similar or identical structures in each generation to keep a rich diversity of structure in the population, and adjusting structures according to the possible space groups to skip the noise on the energy surface, are introduced herein to improve the GAs performance. Furthermore, the application of coevolution strategy between atomic positions and unit cell sizes and shapes *via* the local minimizer greatly reduces the computational cost. This has displayed an improvement in the quality of results found for the theoretical prediction of simple model crystal structures. The performance of the method is illustrated by successful identifications of known carbon and silicon carbide systems, but also gives some new promising structures (*e.g.*, 2D structures). The high success rate of prediction demonstrates the dependability of this methodology and indicates the great potential of our method as a useful technique on crystal structure prediction.

Key words: Genetic Algorithm; Structure Prediction; 2D Material;

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