Adaptive Genetic Algorithm Method for Crystal Structure Prediction and Materials Discovery

C. Z. Wang

Ames Laboratory USDOE and Department of Physics,
Iowa State University, Ames, IA 50011, USA.

The urgent demand for new energy technologies has put great pressure on the capabilities of today's materials and chemical research. Accurate and fast computational structure/property determinations can complement the traditional experimental try and error efforts in material design and accelerate the pace of technological advances. We have recently developed a fast and efficient method for crystal structure prediction and materials discovery. Our method performs genetic algorithm (GA) searches using auxiliary classical potentials to screen the energies of candidate structures, and select only a few of them for more extensive first principles evaluation. Parameters of the auxiliary potentials are adaptively adjusted to reproduce the first-principles results during the course of the GA search. Therefore, the adaptive GA method can have the speed of empirical potential searches but with the accuracy of first principles calculations. The efficiency of the adaptive GA method allows a great increase in the size and complexity of systems that can be studied. We will present results on applications to various systems including metallic alloys and ultrahigh pressure SiO_2, H_2O and Mg-Si-O systems.

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Contact: wangcz@ameslab.gov