Abstract Submitted
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Adaptive Genetic Algorithm method for Crystal Structure Prediction and Materials Discovery[1] CAI-ZHUANG WANG, MIN JI, SHUNQING WU, Ames Laboratory, Iowa State U, Ames, Iowa 50011, KOICHIRO UMEMOTO, U of Minnesota and Ames Laboratory, Iowa State U, RENATA WENTZCOVITCH, Univ of Minnesota, KAI-MING HO, Ames Laboratory, Iowa State U, Ames, Iowa 50011, AMES TEAM[2], MINNESOTA TEAM[3] — We developed a fast and efficient method for crystal structure prediction and materials discovery. The method is based on the cut-and-paste genetic algorithm (GA) scheme introduced by Deaven and Ho [1]. In the evaluation of energies of target structures, first-principles calculations are accurate but time-consuming. Our method performs GA searches uses auxiliary model potentials to screen the energy of candidate structures, selecting only a few 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. Our method combines the speed of empirical potential searches with the accuracy of first principles calculations. We will present results on applications to various systems including metallic alloys and ultrahigh pressure SiO_2, H_2O and Mg-Si-O systems.

[1] D. M. Deaven, K. M. Ho, Phys. Rev. Lett. 75, 288 (1995).

[1]USDOE BES
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