Atomic Structure Prediction with Large-Scale High Performance Computing CAI-ZHUANG WANG, BRUCE HARMON, MANH CUONG NGUYEN, XIN ZHAO, KAI-MING HO, Ames Lab, US DOE, AMES LAB, US DOE TEAM — Many unknown binary or ternary materials for energy applications have very complex crystal structures, containing large number of atoms in their unit cells and possible uncertainty in composition. Computational prediction for atomic structures of such complex materials is a highly demanding work. Advances in modern large-scale high performance computational resources and computational algorithms now make it feasible to perform an efficient crystal structure prediction. We developed an adaptive genetic algorithm to perform large-scale structure search on high performance supercomputer. Examples of successful structure prediction/solving of complex materials will be presented. Further applications of the adaptive genetic algorithm to aid material discoveries will be discussed.

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