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Materials for Alternative Energies: Computational Materials Discovery and Crystal Structure Prediction
CHRIS WOLVERTON, Northwestern University

Many of the key technological problems associated with alternative energies may be traced back to the lack of suitable materials. The materials discovery process may be greatly aided by the use of computational methods, particular those atomistic methods based on density functional theory. In this talk, we present an overview of recent work on energy-related materials from density-functional based approaches. We have developed novel computational tools which enable accurate prediction of crystal structures for new materials (using both Monte Carlo and Genetic Algorithm based approaches), materials discovery via high-throughput, data mining techniques, and automated phase diagram calculations. We highlight applications in the area of Li battery materials and hydrogen storage materials.