Progress from the Methods Development Effort of the Center for the Predictive Simulation of Functional Materials

The Center for the Predictive Simulation of Functional Materials (cpsfm.ornl.gov) aims to develop, apply, validate, and disseminate parameter-free methods and open source codes to predict and explain the properties of functional materials for energy applications. In this talk I will present several aspects of our research, including the development effective core potentials for many body methods, understanding the nature of electronic excitations using variational Monte Carlo and developing systematically improvable approximations applicable to diffusion Monte Carlo in condensed matter.