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Predicting complex materials properties with first principles calculations

We will focus on predictions of the chemical and physical properties of complex

materials for energy applications, including solar, photo-electrochemical and thermoelectric energy conversion. We will discuss two intertwined questions: what is the impact of microscopic theories and first principles simulations on energy related problems? How do we take up the challenge of building much needed tighter connections between computational and laboratory experiments?

Thursday, May 29th 10:00 AM KCBD 1103

http://ime.uchicago.edu/