PHYSICAL CHEMISTRY SEMINAR

Tuesday **11:00 a.m.** **Room 1315**
January 27, 2015 **Chemistry**

Predictive modeling of complex materials from first-principles

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I will present an overview of our efforts to enable predicative atomistic modeling of complex, energy-relevant materials from first-principles. In the first case study, I will describe our recent work examining nano-porous metal-organic frameworks (MOF) materials for gas adsorption and separation applications, with a particular focus on CO2/N2 separations for carbon capture applications. I will also show how our novel force field development methodologies can be generalized to enable unprecedented accuracy in wide variety molecular simulations, with applications ranging from gas phase clusters, to simple liquids, to complex ionic liquids. In the second case study, I will discuss our efforts to develop and apply realistic models for heterogeneous catalysts. By including some of the "complexities" present in working heterogeneous catalysts (e.g. oxide support effects, promoter species) within our models, we are able to help develop a predictive understanding of the influence of these factors. In addition, I will also discuss our recent efforts to design novel computational approaches for analyzing bonding in heterogeneous catalytic systems in a chemically-intuitive manner and thus help establish and important intellectual bridge between traditional homogeneous and heterogeneous catalysis.