



## Department of Chemical Engineering

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### **Predictive and fast: new first-principles tools for materials and catalyst design**

**Thursday, December 13, 2012**

**▶ 9:00 a.m. ◀**

**▶ 321 Morey Hall ◀**

Rational, computational design is a promising path to the development of novel materials and catalysts that can have far-ranging impact from improvements in human health to efficient utilization of energy and resources, but these approaches are often limited by the predictive capabilities and applicable system size of the computational methods employed. I will introduce advances in accuracy and efficiency of electronic structure methods that I have developed that aim to bridge this gap in design strategies through improving upon standard approximations in practical density functional theory and in rethinking hardware and algorithms that we use in order to drastically speed-up simulations. I will show how the first set of improvements reduce errors in descriptions of transition metals critical to both biocatalysis and materials science through examples in non-heme iron metalloenzymes and in self-assembled monolayers of cobalt porphyrins on metallic surfaces, respectively. I will also briefly discuss how hardware-accelerated quantum chemistry can provide unique insight into the geometric and electronic structure of proteins relevant to understanding biocatalysis and developing new catalysts and biomaterials.