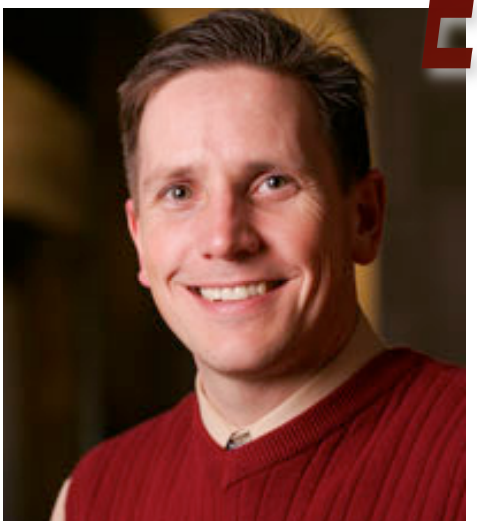
Physical Chemistry Seminar

Tuesday, January 19, 2010 | **11:00 a.m.** | **Room 1315 Chemistry Building**



Environmental Catalysis from First Principles

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Heterogeneous catalysis enabled a revolution in the 20th century in terms of mankind's ability to turn mother nature's materials into useful products for society. In most cases, these applications have preceded rather than followed detailed understanding of catalytic materials and mechanisms. In order to meet the increasing demands of energy sustainability and environmental protection, catalysis science and application in the 21st century has to be driven by basic insights into how materials function and how they can be improved. The advent of first-principles simulations based on density functional theory (DFT), which are able to reliably simulate chemical structures and reactions at the molecular scale, has been instrumental in the recent renaissance in heterogeneous catalysis research. In this talk, I will illustrate the capabilities and challenges of applying these simulation tools in the context of the catalytic chemistry of nitrogen oxides (NO_x). NO_x is an unwanted by-product of combustion and is particularly difficult to remove from lean combustion sources, such as diesel engines. NO_x also has rather complex chemistry that presents special challenges to simulation. I will describe some of our successes in understanding NO_x chemistry from first-principles, with a particular emphasis on recent work to capture the essential features of the beguiling simple catalytic oxidation of NO to NO_2 in molecular models, to reconcile these models with experimental results, and to use these insights to guide the selection of new and improved catalysts.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students may meet with the speaker at 1:15 p.m. in Room 8305f