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# Department of Chemistry

## Seminar

4 p.m. Monday, October 5, 2015 • 331 Smith Hall



Professor

### Sharon Hammes-Schiffer

Department of Chemistry  
University of Illinois

#### *Proton-Coupled Electron Transfer in Catalysis and Energy Conversion*

Research centers on the development and application of theoretical and computational methods for describing chemical reactions in condensed phases and at interfaces. The group is divided into three general areas: proton-coupled electron transfer reactions, enzymatic processes, and non-Born-Oppenheimer electronic structure methods. An overall objective is to elucidate the fundamental physical principles underlying charge transfer reactions.

Website: [http://www.chemistry.illinois.edu/faculty/Sharon\\_Hammes\\_Schiffer.html](http://www.chemistry.illinois.edu/faculty/Sharon_Hammes_Schiffer.html)

#### Abstract

Proton-coupled electron transfer (PCET) reactions play a vital role in a wide range of chemical and biological processes. This talk will focus on recent advances in the theory of PCET. The quantum mechanical effects of the active electrons and transferring proton, as well as the motions of the proton donor-acceptor mode and solvent or protein environment, are included in a general theoretical formulation. This formulation enables the calculation of rate constants and kinetic isotope effects for comparison to experiment. Applications to PCET reactions in solution, enzymes, and electrochemical systems will be presented. Studies of the enzyme soybean lipoxygenase provide a physical explanation for the experimental observation of unusually high kinetic isotope effects for C-H bond activation at room temperature. Investigations of molecular electrocatalysts for hydrogen production identify the thermodynamically and kinetically favorable mechanisms and guide the theoretical design of more effective molecular electrocatalysts. In addition, recent developments of theoretical approaches for simulating the ultrafast dynamics of photoinduced PCET will be discussed. These calculations provide insights into the roles of proton vibrational relaxation and nonequilibrium solvent dynamics in photoinduced PCET processes.

Host: Professor Laura Gagliardi  
Refreshments will be served prior to the seminar.