
J. Clarence Karcher

Lecture

◆DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY ◆THE UNIVERSITY OF OKLAHOMA
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We Are Pleased to Announce a Seminar
Presented by

Sharon Hammes-Schiffer
Yale University

Friday, September 8, 2023
4:00 pm
N'WC 1313

Proton-Coupled Electron Transfer in Catalysis and Energy Conversion

Proton-coupled electron transfer (PCET) reactions play a vital role in a wide range of chemical and biological processes. This talk will summarize the main concepts from our PCET theory and will present applications to catalysis and energy conversion. Our general theoretical formulation for PCET includes the quantum mechanical effects of the electrons and transferring protons, as well as the motions of the donor-acceptor modes and solvent or protein environment. This PCET theory enables the calculation of rate constants and kinetic isotope effects for comparison to experiment and the study of nonequilibrium dynamics. Applications to PCET in enzymes, molecular electrocatalysts, proton wires, nanoparticles, heterogeneous electrochemical systems, and photoreceptor proteins will be discussed. These theoretical studies have identified the thermodynamically and kinetically favorable mechanisms, as well as the roles of hydrogen tunneling, excited vibronic states, reorganization, electrostatics, and conformational motions. The resulting insights are guiding the design of more effective catalysts and energy conversion devices.

(Biography on back.)

Refreshments will be served at 3:45 pm

Dr. Sharon Hammes-Schiffer is the Sterling Professor of Chemistry at Yale University and will move to Princeton University in January 2024. She obtained her Ph.D. degree from Stanford University, carried out postdoctoral research at Bell Laboratories, and then embarked on an extraordinary academic career. Her work in the field of Theoretical and Computational Chemistry, especially the modeling of proton-coupled electron transfer processes in chemistry and biology, has been recognized by her election to the National Academy of Sciences, International Academy of Quantum Molecular Sciences, American Association of the Advancement of Science, and American Academy of Arts and Sciences. Her numerous awards include the American Chemical Society Award in Theoretical Chemistry, National Institutes of Health MERIT Award, and the International Academy of Quantum Molecular Sciences Award. She is the Editor-in-Chief of Chemical Reviews, and serves on the board of reviewing editors of the Science journal and the editorial board of the Proceedings of the National Academy of Sciences, as well as the Editorial Advisory Board of Accounts of Chemical Research, Journal of Chemical Theory and Computation, and the Journal of Physical Chemistry.