

## November 2008 General Meeting - Akron Section Award

Last Updated Sunday, 30 November 2008

Our November meeting will be held on Tuesday, Nov. 11 and will feature the 2008 Akron Section Award winner, Dr. Sharon Hammes-Schiffer, Eberly Professor of Biotechnology & Professor of Chemistry at The Pennsylvania State University. Dr. Hammes-Schiffer will present both an afternoon lecture as well as an evening program. The Akron Section Award is given annually to young scientists who show exceptional promise in his/her career. Abstracts for both talks as well as a short bio can be found by clicking on the "read more" link below.

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Afternoon Seminar

Room 111, Mary Gladwin Hall, The University of Akron

3:30 p.m. "Proton-Coupled Electron Transfer in Solution, Proteins, and Electrochemistry "

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Evening Program

Tangier

5:30 p.m. Networking/Social Time

6:30 p.m. Dinner - Members & Guests - \$17; Students - \$5

7:30 p.m. Program "How Do Biological Enzymes Work?"

The seminar and program are free and open to the public. Dinner reservations are required by noon on Friday, November 7 - please contact Ann Bolek at 330-972-6264 or boleka@uakron.edu.

Afternoon Lecture

Proton-Coupled Electron Transfer in Solution, Proteins, and Electrochemistry

Proton-coupled electron transfer reactions will be examined from the perspective of a general theoretical formulation. The quantum mechanical effects of the active electrons, transferring proton, and donor-acceptor mode, as well as the dynamical effects of the donor-acceptor mode and solvent or protein environment, are included in this formulation. Analytical nonadiabatic rate expressions have been derived in various limits. This approach enables the calculation of rates and kinetic isotope effects, as well as the temperature and pH dependence, for comparison to experiment. Applications of this formulation to solvated metal complexes, tyrosine oxidation in water, and the lipoxxygenase enzyme will be discussed. The extension of this theory to electrochemical proton-coupled electron transfer at metal-solution interfaces will also be presented.

Abstract - Evening Talk

How Do Biological Enzymes Work?

Computer simulations of enzyme reactions provide insight into the mechanism at the atomic level. Methodology has been developed to calculate the reaction rates for comparison to experiment and to make predictions. These simulations also elucidate the role of the structure and dynamics of the enzyme, as well as the impact of enzyme mutations. This talk will

review the insights gained from enzyme simulations with a special focus on the role of protein motion in enzyme reactions. Simulations have provided evidence of a network of coupled motions that extends throughout the enzyme and represents conformational changes that facilitate the catalyzed chemical reaction. Mutations distal to the active site have been shown to significantly impact the catalytic rate by altering the conformational motions of the entire enzyme and thereby changing the probability of sampling conformations conducive to the catalyzed reaction. This type of network has important implications for protein engineering and drug design.

Bio - Sharon Hammes-Schiffer

Sharon Hammes-Schiffer received her B.A. in 1988 from Princeton University and earned her Ph.D. in Chemistry at Stanford University in 1993. After obtaining her Ph.D., she spent the subsequent two years at AT&T Bell Laboratories as a postdoctoral research scientist. In 1995, she accepted a position as the Clare Boothe Luce Assistant Professor of Chemistry and Biochemistry at the University of Notre Dame. In 2000, she accepted a position as the Shaffer Associate Professor of Chemistry at Pennsylvania State University and was promoted to the position of Full Professor of Chemistry in 2003. She was appointed as the Eberly Professor of Biotechnology in 2006. Dr. Hammes-Schiffer's research centers on the investigation of proton and electron transfer reactions in chemical and biological processes. Her work encompasses the development of analytical theories and computational methods, as well as applications to a wide range of experimentally relevant systems. To simulate enzyme reactions, her group has developed a hybrid quantum/classical molecular dynamics approach. These simulations have provided insights into the roles of hydrogen tunneling and protein motion, as well as the impact of distal mutations. Her group has also contributed to the theory of proton-coupled electron transfer reactions in solution, proteins, and electrochemistry. In addition, her group has developed the nuclear-electronic orbital approach for including the quantum effects of selected nuclei in electronic structure calculations. A recent direction of her research is the development of electron-proton density functionals in multicomponent density functional theory. Dr. Hammes-Schiffer's awards include a National Science Foundation CAREER Award, a Ralph E. Powe Junior Faculty Enhancement Award from Oak Ridge Associated Universities, an Alfred P. Sloan Research Fellowship, and a Camille Dreyfus Teacher-Scholar Award. She was selected as an Alexander M. Cruickshank Lecturer for the Gordon Research Conference on Isotopes in Biological & Chemical Sciences in 2004 and was the recipient of both the Iota Sigma Pi Agnes Fay Morgan Research Award and the International Academy of Quantum Molecular Science Medal in 2005. Dr. Hammes-Schiffer has been a Senior Editor for The Journal of Physical Chemistry since 2001. She is a member of the Editorial Advisory Boards for Theoretical Chemistry Accounts, Accounts of Chemical Research, and the Journal of the American Chemical Society. She has also served as Chair of the Theoretical Subdivision of the American Chemical Society and will serve as Chair of the Physical Division of the American Chemistry Society in 2011. Dr. Hammes-Schiffer has over 105 scientific publications and 170 invited talks.