

**DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL  
SCIENCE  
VIRTUAL SEMINAR SERIES  
SPRING 2021**

**DATE:** WEDNESDAY, FEBRUARY 3

**TIME:** 12:30-1:50pm

**LOCATION:**

<https://njit.webex.com/njit/j.php?MTID=mdfe4f718778e9a7ffb4eefa8ea5acb98>

Meeting number: 1202085541

Meeting password: yaP9itPpR74

**Join by video system:**

Dial [1202085541@njit.webex.com](tel:1202085541)

You can also dial 173.243.2.68 and enter your meeting number

**Join by phone:**

1-650-479-3207 Call-in toll number (US/Canada)

**GUEST SPEAKER**

Sharon Hammes-Schiffer  
Department of Chemistry  
Yale University  
New Haven, CT

**TOPIC**

Proton-Coupled Electron Transfer in Catalysis and Energy Conversion

**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 and applications to catalysis and energy conversion. 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. Recent extensions enable the study of heterogeneous as well as homogeneous PCET processes. Applications to PCET in enzymes, molecular electrocatalysts, proton wires, photoreduced zinc-oxide nanocrystals, and proton discharge on gold electrodes will be discussed. In addition, recent developments of theoretical approaches for simulating the ultrafast nonequilibrium dynamics of photoinduced PCET, along with applications to photoreceptor proteins, will

be discussed. Overall, these studies have identified the thermodynamically and kinetically favorable mechanisms, as well as the roles of proton relays, excited vibronic states, hydrogen tunneling, reorganization, electrostatics, and conformational motions. The resulting insights are guiding the design of more effective catalysts and energy conversion devices.

### **BIO**

Sharon Hammes-Schiffer received her B.A. in Chemistry from Princeton University in 1988 and her Ph.D. in Chemistry from Stanford University in 1993, followed by two years at AT&T Bell Laboratories. She was the Clare Boothe Luce Assistant Professor at the University of Notre Dame from 1995-2000 and then became the Eberly Professor of Biotechnology at The Pennsylvania State University until 2012, when she became the Swanlund Professor of Chemistry at the University of Illinois Urbana-Champaign. Since 2018, she has been the John Gamble Kirkwood Professor of Chemistry at Yale University. She is a Fellow of the American Physical Society, American Chemical Society, American Association for the Advancement of Science, and Biophysical Society. She is a member of the American Academy of Arts and Sciences, the U.S. National Academy of Sciences, and the International Academy of Quantum Molecular Science. She has received the American Chemical Society Award in Theoretical Chemistry, the Gibbs Medal Award, the Royal Society of Chemistry Bourke Award, and the Joseph O. Hirschfelder Prize in Theoretical Chemistry. She is currently the Editor-in-Chief of *Chemical Reviews* and is on the Board of Reviewing Editors for *Science*. She has over 300 publications and has given more than 430 invited lectures.

### **Committee members:**

**Professor Michael Eberhart – [michael.s.eberhart@njit.edu](mailto:michael.s.eberhart@njit.edu)**  
**Professor Farnaz Shakib – [farnaz.a.shakib@njit.edu](mailto:farnaz.a.shakib@njit.edu)**