



# Emerson Center Lectureship Award Symposium

## Proton-Coupled Electron Transfer in Biology, Catalysis and Energy Conversion

April 21, 2022

Department of Chemistry,  
Atwood Hall, Room #360

**AWARD WINNER &  
KEYNOTE SPEAKER**

**Prof. Sharon Hammes-Schiffer,  
Yale University**

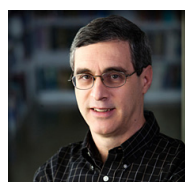
### Proton-Coupled Electron Transfer in Catalysis and Energy Conversion



Proton-coupled electron transfer (PCET) reactions play a vital role in a wide range of chemical and biological processes. The quantum mechanical formulation includes the effects of the active electrons and protons, as well as the motions of the donor-acceptor modes and solvent or protein environment. Roles of PCET in enzymes, molecular electrocatalysts, nanoparticles, proton discharge on electrodes, and photoreceptor proteins will be discussed. Our 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.

#### INVITED SPEAKERS

#### EVENTS SCHEDULE



**Brian Dyer**  
Department of  
Chemistry,  
Emory University

1:30 – 2:00

**OPENING CEREMONY & AWARD PRESENTATION**

2:00 – 3:00

**Sharon Hammes-Schiffer:**  
**Proton-Coupled Electron Transfer in Catalysis  
and Energy Conversion**

3:00 – 3:50

**Brian Dyer: Proton Coupled Electron  
Transfer in Hydrogenase Enzymes**



**Tim Lian**  
Department of  
Chemistry,  
Emory University

3:50 – 4:00

**COFFEE BREAK**

4:00 – 4:50

**Tim Lian: Probing the catalyst microenviron-  
ment at electrode/liquid interface by surface  
selective vibrational spectroscopy**



**Kurt Warncke**  
Department of  
Physics,  
Emory University

4:50 – 5:30

**Kurt Warncke: Select Protein and Coupled  
Solvent Dynamics in Enzyme Catalysis**

5:30 – 5:45

**CLOSING**

6:00 – 9:00

**DINNER (by invitation)**

**Go-  
SPONSORS:**



**DEPARTMENT OF CHEMISTRY  
THE HIGHTOWER FOUNDATION;**

**REGISTRATION:**

<http://www.emerson.emory.edu/conferences/form/register.html>

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*Registration is free.*