



# 2021-22 JOSEPH O. HIRSCHFELDER LECTURES IN THEORETICAL CHEMISTRY

Wednesday, September 15, 2021 at 3:30 p.m.  
Social Sciences Building, Room 5106  
1180 Observatory Drive  
Hosts: Professors Ned Sibert and JR Schmidt

**Professor Sharon Hammes-Schiffer**  
**John Gamble Kirkwood Professor of Chemistry**  
**Department of Chemistry**  
**Yale University**

## **INTEGRATING ELECTRONIC AND NUCLEAR QUANTUM EFFECTS VIA THE NUCLEAR-ELECTRONIC ORBITAL APPROACH**

Nuclear quantum effects such as zero point energy, nuclear delocalization, and tunneling play an important role in a wide range of chemical and biological processes. The incorporation of nuclear quantum effects and non-Born-Oppenheimer behavior into quantum chemistry calculations and molecular dynamics simulations is a longstanding challenge. To address this challenge, the nuclear-electronic orbital (NEO) approach treats specified nuclei, typically protons, quantum mechanically on the same level as the electrons with multicomponent density functional theory (DFT) or wave function methods. This approach inherently includes nuclear delocalization and zero-point energy in molecular energy calculations, geometry optimizations, reaction paths, and dynamics. It can also provide accurate descriptions of excited electronic, vibrational, and vibronic states, as well as nuclear tunneling and nonadiabatic dynamics. The real-time NEO methods enable nonequilibrium nuclear-electronic dynamics simulations beyond the Born-Oppenheimer approximation for the investigation of excited state chemical reactions. This talk will provide an overview of the foundational NEO methods as well as applications to photoinduced proton transfer and hydrogen tunnelling processes.

FOR MORE INFORMATION, CONTACT:  
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