

Department of Chemistry Seminar

Dr. Micheline Soley

Yale University



Monday, January 24 at 3:30 PM (CT)

Virtual Event

Host: Prof. Randy Goldsmith

“From Ultracold Chemistry to Quantum Computing: Chemical Reactions Under Quantum Control”

Molecules below one milliKelvin are currently of intense interest given the insight they offer into chemical reactions at the level of individual states and their ability to serve as qubits in molecule-based quantum computers. For the past thirty years, both quantum scattering and dynamics calculations have been plagued by the fact the technique often generates unphysical reflection of low-energy components of wave packets. I will introduce a physical, semiclassical solution I developed based on classical trajectories and will demonstrate the method reduces anomalous reflection by several orders of magnitude relative to the standard approach and provides a solution to the decades-old problem posed by complex absorbing potentials. In addition, I will discuss a method inspired by optics, which I developed to advance targeted product formation in ultracold chemistry. The method drives low-energy reactions to form product molecules with zero reformation of reactants, while requiring no more than two control parameters. To conclude, I will discuss quantum computing approaches I have developed for molecular geometry optimization and dynamics simulations in chemistry, both on today's quantum computers and on classical computers with the use of data-compressed tensor networks/matrix product states.

For more information, contact: Irena Garic at garic@wisc.edu



Department of Chemistry
UNIVERSITY OF WISCONSIN-MADISON