



Department of Physics Colloquium

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3:00 PM



Quantum Dynamics of Ultracold Chemical Reactions: Quantum Interference, Excited Electronic States, and Long-lived Complexes

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Experimental techniques for cooling, trapping, and colliding cold ($T < 1$ K) and ultracold ($T < 1$ mK) molecules continue to develop at an astounding pace. Recent techniques using external fields and/or initial quantum state selection have demonstrated exquisite control of the collision outcome including chemical reactions. Recent experiments have also identified reaction intermediates (also known as metastable states or complexes) and have measured their lifetimes. For Rb colliding with KRb these lifetimes exceed simple theoretical estimates by five orders of magnitude! Thus, an accurate theoretical treatment of ultracold chemical reactions is needed for the understanding of the reaction mechanisms and interpreting the experimental measurements. However, accurate calculations are challenging and require a fully quantum mechanical first-principles description of the both the electronic and nuclear motion. A numerically exact quantum reactive scattering methodology for atom-diatom ($A + BC$) collisions/reactions will be reviewed. This methodology is ideally suited for treating ultracold chemical reactions and has recently identified a novel quantum interference mechanism that could be exploited to effectively turn the chemical reaction on or off (i.e., a quantum molecular switch!). This mechanism is general and has been shown to occur in a variety of ultracold chemical reactions: $O + OH \rightarrow H + O_2$, $H + HD \rightarrow H + HD$ (and isotopic variants), and $Li + LiNa \rightarrow Li_2 + Na$. Of particular interest is the crucial role of an excited electronic state that becomes degenerate with the ground electronic state. The geometric phase associated with this degeneracy is shown to control the constructive or destructive nature of the quantum interference and hence the reaction outcome. For many ultracold reactions, the excited electronic state is energetically accessible even at ultracold collision temperatures. Thus, a fully coupled two-electronic state (non-adiabatic) calculation is required. The excited electronic state can also lead to very long-lived reaction complexes that could be the origin of the experimentally observed lifetimes for Rb + KRb.

**This colloquium will be held in-person, at SERC 116
unless announced otherwise.**