UCLA College | Physical Sciences Chemistry & Biochemistry

PHYSICAL CHEMISTRY SEMINAR

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4:00 PM
Young Hall 2033

"Quantum Resonances in Molecular Systems at High Energy: Cold Collisions of Hot Molecules and Quantum Roaming Dynamics"

Abstract: There is keen interest now in novel chemistry in the cold and ultracold regime where quantum effects are expected to dominate and interactions are largely controlled by resonances. Considering these issues we are led to ask: what happens when these interactions involve excited molecules, perhaps at half an eV? Or even 4 eV? What happens when multiple continua can interact? When might resonances play an important role, or simply one that we can tease out of a classical-looking average? I will present two different sets of experiments in which we explore these questions. In the first, we combine stimulated emission pumping with velocity map imaging for the first time to study cold collisions of nitric oxide prepared in single quantum states of v=10. We perform these studies in a novel near-copropagating beam configuration that gives broad control over the collision energy from above room temperature down to 1 K. We explore a region where the attractive potential dominates the interaction, and demonstrate control over the product differential cross sections. The results are compared to quantum scattering calculations on a variety of high-level potential energy surfaces and we find the results offer a serious challenge to theory, particularly for cold, spin-orbit quenching collisions. I will then turn to an investigation of the roaming radical reaction pathway ¬– in which a molecule undergoes near-dissociation to radicals followed by reorientation and intramolecular reaction at long range – seeking evidence of quantum effects. We will show dramatic evidence of the emergence of quantum orbiting resonances in a detailed study of formaldehyde photodissociation that profoundly modulate the roaming yield over a narrow energy range, and reveal strong coupling between the roaming, radical and conventional dissociation pathways in this system. The results are interpreted with the aid of quantum dynamics calculations in reduced dimensionality. Together these two systems highlight the fact that quantum resonances can strongly influence the dynamics even in systems at high total energy.

Please contact marla@chem.ucla.edu for additional information.