

Nonadiabatic Transitions via Conical Intersections in Ultracold Chemical Reactions

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Collisions and reactions among atoms, ions and small molecules can now be investigated at temperatures well below 1 mK. Here, quantum effects, such as threshold phenomena, can not be ignored. In this presentation, I will discuss our recent results on ultracold atom-molecule reactivity, focussing on heteronuclear polar molecules, where intermediate short-range complexes with conical intersections are important. Conical intersections correspond to geometries where two potential energy surfaces touch. Nonadiabatic passage through these intersections causes a breakdown of the Born-Oppenheimer approximation that strongly affects molecular dynamics and the chemical properties of molecules. I will also discuss control of ultracold charge exchange among an atom and an atomic ion in the presence of a strong cw laser field. The laser induces a conical intersection and strong non-adiabatic transitions.

Our simulations have required us to perform electronic structure calculations of the multi-dimensional potential energy surfaces of ground and excited states for both short- and long-range internuclear geometries. We located and determined properties of CIs as well as extracted the three-body non-additive contribution to the potentials. We also performed coupled-channels computations based on a first-principles description of the collisional dynamics and determined total reaction rate coefficients as well state-to-state resolved product distributions. We interpret the outcomes in terms of random matrix theory.