The Polyatomic Dynamics of Electron-Driven Chemistry

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Electron collisions with atoms and molecules initiate almost all the relevant chemistry associated with the plasma processing of materials, radiation chemistry and modern lighting technology. In the life sciences, the dissociative attachment of low energy electrons has been implicated in the initiation of strand breaking in DNA. The treatment of the polyatomic dynamics of electron-driven chemistry from first principles has finally been made possible by a combination of advances in theoretical techniques for electron-molecule scattering with modern wave packet methods for describing the nuclear dynamics of polyatomic molecules. This talk will discuss the ways in which the multidimensional nuclear dynamics in polyatomic systems during resonant electron collisions result in the channeling of electronic energy into vibrational excitation and dissociation, and how those dynamics can produce effects that cannot be described by one-dimensional models. The state of the art will be illustrated by calculations on dissociative attachment of electrons to water in full dimensionality, $e^- + H_2O \rightarrow \begin{cases} H^- + OH \\ O^- + H_2 \end{cases}$.

This example also illustrates how the dynamics on the potential surfaces associated with multiple resonances can be affected by conical intersections between them that may determine which dissociation products will be produced.