

Creativity in Science: Theoretical Predictions in Chemical and Biological Physics

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Electron-molecule collisions have been found to play a crucial role in the radiation damage of biological molecules. Electrons also drive many of the atomic and molecular processes in planetary upper atmospheres and initiate most of the relevant physics and chemistry associated with the plasma processing of materials for microelectronics and modern electric lighting technology. In spite of the importance of these fundamental processes, relatively little is known about them. Only components of the fundamental physics are well understood, and only a few of the required cross sections and rates for the multitude of important molecules are known with confidence. At a larger scale, we are seeking a thorough understanding of the mechanisms that take place at the molecular level and that are associated with the function and disease of biological molecules.

This talk will give a short introduction to some of the important fundamental processes in electron-driven processes and the theory needed to describe them in a predictive manner. It will also give an overview of how calculations can help us understand the dynamics of biological molecules. I will present results of a complete ab initio study of vibrational excitation and dissociative electron attachment to nitric oxide that illustrate the predictive power of our computational treatment of these processes. I will discuss a prime example that exhibits much of the complexity of electron-driven chemical and physical processes on polyatomic molecules by reporting our findings on dissociative electron attachment to the simplest organic acid: formic acid. I will also show how simulations are helping us elucidate the mechanisms by which proteins bind metal ions and how this process may lead to the disruption of structures that are associated with neurodegenerative diseases.