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Electron Collisions with Large Molecules¹

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In recent years, interest in electron-molecule collisions has increasingly shifted to large molecules. Applications within the semiconductor industry, for example, require electron collision data for molecules such as perfluorocyclobutane, while almost all biological applications involve macromolecules such as DNA. A significant development in recent years has been the realization that slow electrons can directly damage DNA. This discovery has spurred studies of low-energy collisions with the constituents of DNA, including the bases, deoxyribose, the phosphate, and larger moieties assembled from them. In semiconductor applications, a key goal is development of electron cross section sets for plasma chemistry modeling, while biological studies are largely focused on understanding the role of localized resonances in inducing DNA strand breaks. Accurate calculations of low-energy electron collisions with polyatomic molecules are computationally demanding because of the low symmetry and inherent many-electron nature of the problem; moreover, the computational requirements scale rapidly with the size of the molecule. To pursue such studies, we have adapted our computational procedure, known as the Schwinger multichannel method, to run efficiently on highly parallel computers. In this talk, we will present some of our recent results for fluorocarbon etchants used in the semiconductor industry and for constituents of DNA and RNA. In collaboration with Carl Winstead, California Institute of Technology.

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