Electron Collisions with Molecules and Molecular Clusters

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Electron scattering data requirements in a variety of fields (astrophysics, plasma modelling, medical physics, etc.) have provided significant impetus to the study of electron-molecule collision over the last couple of decades. A case in point is the need to understand how low energy electrons generated by ionizing radiation in a biological medium cause damage to cell constituents [1]. This stimulus has led to the further development of theoretical approaches to treat electron-molecule scattering as well as the reengineering of many of their software implementations. Some of these developments have wider application, as the need to model correlated multielectronic effects that involve the continuum in molecules is also present in the study of molecular photoionization, strong-field process, etc. [2].

The work carried has allowed the accurate computation of cross sections and the investigation of resonance formation [3] for larger targets than ever before as well as high quality calculations for smaller targets. These larger targets include small molecular clusters [4]: their study aims at bridging the gap between the pure gas phase and the actual condensed environment in which many of the collisions of applied relevance take place. Developments have also contributed to improving our fundamental understanding of electron scattering from molecules.

In my talk, I will discuss the present successes and future challenges of studying low energy electron scattering computationally, focussing on the application of the R-matrix method [5, 6] to isolated molecules and small molecular clusters.

References

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