Invited: AMOP-I-01

Dynamics of Electron – Molecule Resonances: A Challenge to Computational Physics

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Electron-molecule resonances play a dominant role in electron induced chemistry and hence find crucial role in wide variety of applications ranging from nano lithography to radiation therapy and in other basic sciences. The dynamics of the formation and decay of these resonances decides the nature of products and the subsequent chemistry. Thus understanding these processes in various molecules are necessary for various applications.

The electron-molecule resonances decay through two competing modes – electron ejection and dissociation. The final products are determined by the mixing between the electronic and nuclear degrees of freedom. There has been some success in identifying these resonances in very small molecules by doing scattering calculations using R-matrix or similar codes. In order to follow the dynamics, these scattering calculations have to be coupled to the nuclear dynamics. There has been very limited success so far in this respect. Recent developments in ion momentum imaging [1] have provided a wealth of information on these resonances [2 - 6], allowing crucial tests for theoretical techniques. However, a great deal of these results remains unexplained even for simple diatomic molecules. This talk would cover some of the recent results and highlight how the complex system of electron-molecule resonances still remains a challenge to computational physics.

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