Recent Advances in the Theory of Dissociative Electron Attachment

I. I. Fabrikant[1] and H. Ambalampitiya[1]
[1]Department of Physics and Astronomy, University of Nebraska-Lincoln
ifabrikant@unl.edu

Dissociative electron attachment (DEA) to polyatomic molecules is a complicated process involving couplings between electron and nuclear motion. Completely *ab initio* calculations are presently possible only for diatomics, and model approaches should be developed for more complex targets, particularly if nonlocal effects, leading to vibrational Feshbach resonances (VFR) and threshold cusps, are important [1-3]. In the last few years we have been working on several problems related to DEA to polyatomic molecules:

• Extension of the nonlocal theory to two and more degrees of freedom. The properties of the Green's operator describing the evolution of the resonant state play the crucial role in the nonlocal effects. Quantum-mechanical and semiclassical methods of its calculation have been developed. They can be incorporated in the equivalent resonant R-matrix theory which is more convenient for model calculations. The general theory has been applied to the CF_3Cl compound. DEA to this molecule was studied in the past by one-dimensional nonlocal theory and two-dimensional local theory incorporating symmetric stretch and umbrella vibrations. The present version combines both nonlocal and two-dimensional effects.

• Application of the effective range theory to description of VFRs and threshold cusps in polyatomics. This theory was applied recently to description of cusp structure in DEA to $Fe(CO)_5$ [4], the molecule important for the development of the Free-Electron-Beam Induced Deposition technique, and to a series of 5-membered heterocyclic rings [5].

• Investigation of the role of the water cluster environment in DEA to polyatomics, particularly to biological-relevant molecules like thymine. There are two effects in this process, one leading to the enhancement of the DEA cross section due to the increased lifetime of the intermediate negative-ion state [6], and the other leading to the decrease of the yield of the anionic fragments due to the hydrogen bonding between the nucleobase and the solvent [7].

References
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