SEMINAIRE ISMO

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Recent progress in the theory of dissociative electron attachment: from diatomics to biomolecules

We present a summary of recent progress in theoretical studies of low-energy dissociative electron attachment (DEA) to halogen molecules and polyatomic molecules based on the resonance R-matrix theory. It explains many observed features in DEA cross sections including low-energy behavior, threshold resonances and cusps. It also gives description of the temperature dependence of the attachment rate coefficients. The theory was also applied to several molecules of biological interest: formic acid, glycine, thymine and uracil [1,2]. Particular outstanding features are sharp peaks in DEA cross sections for uracil and thymine, which are interpreted as vibrational Feshbach resonances. More recent calculations describe DEA to alanine, β-alanine, and α-, β- and γ-aminobutanoic acids. We also investigated isotope effect and the results confirm experimental findings [3] for deuterated uracil and thymine.

For practical applications to radiation damage, it is important to know how DEA processes are modified in condensed-matter environments. It is known that the long-range effects are significantly suppressed in this case. A particular interesting example is a suppression of the VFR effect in DEA to the CH_3I molecule observed experimentally [4]. Recent calculations confirm that the cross section for DEA to the CH_3I molecule physisorbed on a surface of the Kr film is reduced by an order of magnitude as compared to the gas phase DEA cross section.

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