Electron-molecule dynamics for non-equilibrium plasmas

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In my presentation, I will illustrate my research on electron-molecule dynamics at ISTP of CNR in Italy. I will focus in particular on vibrational-excitation, dissociative-attachment, dissociative-recombination and dissociative-excitation processes rotationally and vibrationally resolved. The electronic structures are obtained by using ab-initio quantum chemistry approaches implemented in computer codes like MOLPRO and UK–R-Matrix whereas the nuclear dynamics is studied within the theoretical models of Bardsley's local-complex-potential model, adiabatic-nuclei approximation and multichannel quantum defect theory. The latest results for cross sections and rate coefficients will be presented and discussed for ArH^+ [1], BeH^+ [2, 3], H_2, H_2^+, N_2 [4], O_2 [5], CO [6], CO^+, CO_2.

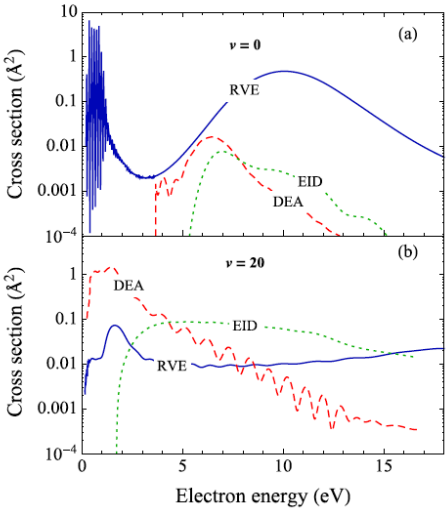

Fig. 1. Summary on electron-O_2 cross sections [5]: vibrational excitation (RVE), dissociative attachment (DEA), and dissociative excitation (EID) processes for the vibrational levels $v = 0$ (a) and $v = 20$ (b).

These researches are performed in view of many applications: in particular in aerospace (shuttle reentry in planetary atmospheres, electric propulsion); non-equilibrium plasma physics (combustion); controlled fusion reactors; astrochemistry (early Universe, interstellar medium) and chemical evolution of life just to name a few. Finally, some kinetics modelling will be also presented.

Results are obtained in collaboration with the groups of I.F. Schneider (France), J. Tennyson (UK) and M. Panesi (US).

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