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\textsuperscript{+} [1], BeH\textsuperscript{+} [2, 3], H\textsubscript{2}, H\textsubscript{2}\textsuperscript{+}, N\textsubscript{2} [4], O\textsubscript{2} [5], CO [6], CO\textsuperscript{+}, CO\textsubscript{2}.

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).