Reactive collisions of electrons with molecular cations: from time-independent to time-dependent approaches

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Electron-impact dissociative recombination (1), ro-vibrational excitation (2) and dissociative excitation (3) [1]:

$$AB^+(N_i^+,v_i^+)+e^- \rightarrow AB^*,AB^{**} \rightarrow A+B, \quad (1)$$

$$\rightarrow AB^*,AB^{**} \rightarrow AB^+(N_f^+,v_f^+)+e^-, \quad (2)$$

$$\rightarrow AB^{**} \rightarrow A+B^+ +e^-, \quad (3)$$

- AB* standing for Rydberg bound states and AB** for dissociative states - occur in various ionized media of astrophysical, energetic and industrial interest.

Being highly-reactive, involving super-excited molecular states undergoing predissociation and autoionization, and having a strong resonant character, these collisions are subject to beyond-Born-Oppenheimer theoretical approaches, and often require quasi-diabatic - rather than adiabatic - representations of the molecular states, as well as particularly sophisticated methods for modelling the fragmentation dynamics, able to manage the superposition of many continua.

I will briefly describe the method that we use the most often to study these reactions, based on the Multichannel Quantum Defect Theory (MQDT), capable to take into account the strong mixing between ionization and dissociative channels, open - direct mechanism - and closed - indirect mechanism, and the capture into infinite series of Rydberg resonances [2-4], with illustrations for H_2^+ [5,6], CH^+ [7], CO^+ [8], N_2^+ [9], SH^+ [10], and H_3^+ [11]. An other time-independent method we used, applied to BeH^+ [12], is based on the Configuration Interaction method and the projector operators technique [13].

The need to predict branching ratios and to address polyatomic systems pushed us to an attempt to use a wave-packet method, which will be illustrated for HD^+ [14]. This attempt should be followed by a more substantial effort in order to apply the MCTDH method to the study of these processes.

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