

Abstract for an Invited Paper
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Theory of dissociative recombination of triatomic molecular ions¹

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In this talk I will discuss several techniques recently developed for the theoretical description of dissociative recombination of molecular ions and related processes such as molecular photoionization and rovibrationally-inelastic electron-collisions with the ions. The techniques are based on quantum defect theory, an efficient tool for characterizing electron-ion collision processes. In order to apply the same theoretical techniques to both diatomic and triatomic ions, we utilize an appropriate adiabatic dissociative coordinate: for diatomic ions it is the internuclear distance, while for triatomic ions it is the hyperradius or some other suitable coordinate representing the dissociative degree of freedom. A unique adiabatic dissociative coordinate is needed in order to treat the dissociative flux escaping into different rovibrational and fragmentation channels in a uniform way. If needed, the approximation of adiabaticity of such dissociative coordinate can be lifted by taking non-adiabatic couplings explicitly into account. I will concentrate on a time-independent theoretical framework that has been applied to describe dissociative recombination in such ions as H_3^+ and its isotopologues (H_2D^+ , D_2H^+ and D_3^+), HCO^+ (DCO^+). I will also discuss the time-dependent framework of the theory to represent dissociation recombination. For the linear triatomic ions with large dipole moment we have modified the approach to include the effect of the dipole moment of the ion on the motion of the incident electron. For this purpose we have applied the multichannel quantum defect theory generalized to deal with the Coulomb field with non-integer complex partial waves.

¹In collaboration with Nicolas Douguet, Samantha Santos, and Chris H. Greene