Theoretical studies of charged particle collisions

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We report on *ab initio* quantum mechanical studies on mutual neutralization in collisions of atomic or molecular ions such as H^-colliding with H^+or H_2^+, where an electron transfer results in the formation in neutral fragments. Results from theoretical studies on mutual neutralization in H^+ and H^- collisions will be reported. Previously [1,2], we have computed the total and differential cross sections and branching ratios at collision energies below 100 eV by considering non-adiabatic radial interactions among the $^1\Sigma_g^+$ as well as the $^1\Sigma_u^+$ states associated with the asymptotic limits of H+H(n≤3) as well as $H^+ + H^-$. Also the double electron transfer has been studied [3]. The limitations of the theoretical model are now tested by including the n=4 states as well as other types of couplings such as rotational couplings between electronic states of different symmetries. New structure calculations on the H_2 system have been performed in order to compute all relevant potentials and coupling elements. Detailed comparisons with measurements are done.

Ab initio studies on collisions of atomic and molecular ions are challenging and preliminary results on $H_2^+ + H^-$ scattering will be reported. Potential energy surfaces and non-adiabatic interactions of highly excited H_3 states in $^2A'$ symmetry are computed using the full configuration interaction method and as can be seen in Figure 1, the electron transfer can be driven by avoided crossings at large H_2 – H distances due to interactions between ionic and covalent states.

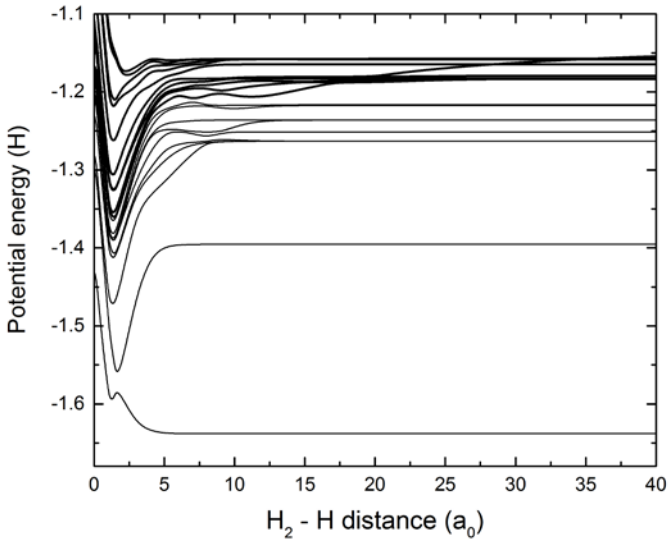

Figure 1: Adiabatic potential energy surfaces of the H_3 system in $^2A'$ symmetry.

[1] Stenrup M et al 2009 Phys. Rev. A **79,** 012713
[2] Nkambule S M et al 2016 Phys. Rev. A, **93**, 032701
[3] Mezei J Zs et al 2010 Phys. Rev. A, **82**, 014701