# Cold and ultracold dynamics of the barrierless reaction $D^+ + H_2$

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The $H_3^+$ system is considered the prototype of barrierless ion-molecule reaction. It has been extensively studied theoretically and experimentally due to its importance in astrochemistry [1]. Below 1.7 eV, the only reactive process that can take place on the ground adiabatic potential energy surface (PES) is the non-charge transfer proton exchange process. We have calculated quantum reactive cross-sections for the collision $D^+$+*para*-$H_2$ $\rightarrow H^+$+HD using the hyperspherical quantum reactive scattering method[2]. Considered kinetic energies range from the ultracold regime, where only one partial wave is open, up to the Langevin regime, where many of them contribute. At very low kinetic energies, long-range (LR) interactions (usually neglected in both PES and dynamics calculations) determine the amount of incoming flux which reaches the short range region where rearrangement may occur, and are thus essential. Both accurate descriptions of the LR region in the PES, and long dynamical propagations, up to distances of hundreds of a.u., are required. Accordingly, the hyperspherical methodology was recently modified in order to allow considering LR interactions while minimizing the computational expense[3]. The method is suitable for systems involving ions, as the $R^{-4}$ behaviour largely extends the range of the potential. Besides, very simple ideas stemming from Multi-Quantum Defect Theory allow methodological tricks which may further reduce the expense[4]. In order to show the significance of the LR effects, calculations are carried out on two different published PES[5], which result from two different fittings of similar *ab initio* points: one fitting does not pay special attention to the LR interactions while the correct LR behaviour is explicitly included in the other.

Emerging experimental techniques are making possible quick advances in the analysis of cold and ultracold reaction dynamics, and the title system appears as a good candidate for such experimental studies. The range of energies where the Wigner regime should be found is discussed.

## References

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