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On the effect of long-range interactions in low-energy collisions

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The basic ingredient needed to properly investigate elementary processes promoted by collisions is the accurate characterization of the interaction potentials. Progress in computational resources and in efficient interpolation procedures has allowed to obtain fast and reliable potential energy surfaces (PES) in the region of strong interaction between the colliding partners. The medium and long-range regions on the other hand often remain neglected or only poorly characterized, a choice justified by the belief that it is the short-range potential to mainly drive the dynamics of elementary processes.

There is however increasing evidence [1,2], like inexplicable discrepancies between calculated and experimental values [3], that the outcome of all collisional events, particularly in the low temperature regime, is strongly determined by the formation of weakly bound complexes or precursor states, which need to be correctly and accurately described. This is a well-known issue for the reliable determination of rate coefficients for inelastic vibrational energy transfer processes [1,4] and turns out to be as well important for the rates of reactive events [5]. From a more fundamental perspective this is bound to be relevant in the modeling and in the critical understanding of low temperature collision physics, where the uncertainty due to the necessity of a quantum vs. a classical treatment of the various degrees of freedom needs to be disentangled from that arising from a poor treatment of long- range effects.

Some case studies, where the accurate formulation of the long-range potential is basic to provide reliable results for low energy (but not only) inelastic and reactive events, will be illustrated, with a particular emphasis on the stereodynamics and anisotropy effects driving the outcome of collisional phenomena.

References

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