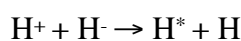


Theoretical studies of scattering processes involving H₂ and BH reaction complexes

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With *ab initio* structure and electron scattering calculations on H₂, a diabatic representation of the excited bound and resonant electronic states have been developed¹. The model allows for inclusion of an arbitrary number of Rydberg states as well as rotational couplings, autoionization and a correct treatment of non-vanishing non-adiabatic couplings. The model is used to perform quantum mechanical studies of different scattering processes involving the same set of electronic states. Total and differential cross section and branching ratios are computed for processes such as mutual neutralization¹



associative ionization²



and dissociative recombination



The calculated results are compared with measurements. The processes are computed for different hydrogen isotopes and different ro-vibrational states of the molecular ion relevant for the fusion plasmas.

A similar diabaticization method will be used to study processes involving the BH reaction complex. Electron structure calculations using the MRCI method have been performed to compute adiabatic potential energy curves of the excited states of BH and BH⁺. The extracted effective quantum numbers are compared with quantum defects obtained from the structure calculations on BH by Petsalakis *et al.*³ Preliminary results from electron scattering calculations using the Complex Kohn variational method was presented. Using the diabatic potentials and couplings, dissociative recombination of BH⁺ will be studied using the MQDT method in collaboration with the groups of I. F. Schneider and Z. Mezei.

¹ J. Hörnquist, P. Hedvall, Å. Larson and A E Orel, Phys. Rev. A, **106**, 062821 (2022).

² J. Hörnquist et al. Phys. Rev. A, **108**, 052811 (2023).

³ I. D. Petsalakis, G. Theodorakopoulos, Mol. Phys. 104, 103, (2006).