Theoretical studies of reactive scattering processes involving the \( \text{H}_2 \) reaction complex

Scattering processes such as mutual neutralization, double charge transfer, associative ionization, dissociative recombination and resonant ion-pair formation involve highly excited states and non-adiabatic effects are therefore crucial. I will present a model that makes it possible to systematically study all of the above processes \textit{ab initio} and fully quantum mechanically using accurate potentials and couplings. More specifically, the model makes it possible to include an accurate description of bound electronic states as well as Rydberg states and electronic resonant states. Furthermore, it includes non-adiabatic couplings between bound electronic states, both at small and large internuclear distances, as well as couplings to resonant states and to the ionization continuum. Results will be presented on an application of the model to the \( \text{H}_2 \) system. The model is not limited to the \( \text{H}_2 \) system and may serve as a basis for which more complicated systems can be studied.