Quantum Dynamics Studies of Chemical Reactions

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Abstract

In this talk, I will present some of our recent work on accurate quantum reactive scattering studies of chemical reactions involving four, and six atoms. For four-atom reactions, I will show the full dimensional differential cross sections for the HD/D_2+OH reactions and for the exchange H + H_2O reaction. Because it is necessary to treat both OH bonds in H_2O as reactive bonds in the exchange reaction, it is much more expensive computationally to study the exchange reactions. For six-atom reactions, I will present some quantum dynamics results for the H/F/Cl+CHD_3 reactions on accurate potential energy surfaces.