Quantum Non-adiabatic Dynamics in Polyatomic Photodissociation

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Photoexcitation to electronically excited manifold sometimes leads to fragmentation, which is often facilitated by the breakdown of the Born-Oppenheimer approximation. As a result, photodissociation of small molecules serves as a proving ground for understanding of non-adiabatic dynamics prevalent in many photo-reactions such as photovoltaic and vision. To gain a quantitative understanding of these processes, one needs a full-dimensional quantum characterization of the dissociation dynamics on accurate global potential energy surfaces as well as their couplings. The merge of these two approaches yields unprecedented insights into these half-collision processes. In this presentation, I will discuss our latest work on quantum dynamics of photodissociation of H_2O in its *B* band on a set of newly developed diabatic potential energy surfaces.[1-3] I will focus on the competing non-adiabatic pathways via the conical intersections and Renner-Teller coupling. In addition, I will also discuss our six-dimensional wave packet studies on the photodissociation of NH_3 and ND_3 in their *A* band using the recent diabatic potential energy surfaces developed by Zhu and Yarkony.[4-7] I will focus on the non-adiabatic dynamics with and without vibrational excitation on the ground electronic state.

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