

화학고 세미나

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POSTECH 화학과

Coherent Chemical Dynamics in Electronic Excited States

Chemical reaction dynamics are generally governed by the underlying potential energy landscape including reaction barriers and thermodynamic driving forces. For reactions that occur on a timescale shorter than vibrational dephasing time, however, coherent nuclear motions can play a significant role, and the reaction may proceed through directed nuclear wave-packet motions. Femtosecond optical pulses shorter than a vibrational period can launch coherent nuclear wave packets in electronically excited states. Their subsequent evolution is governed by the potential energy surfaces and electron–nuclear coupling that drive the reaction.

At early times in a photochemical reaction, nuclear motion can be described in terms of the normal modes of the reactant. Following the reaction, the nuclear motion can instead be projected onto the normal modes of the product. This framework allows us to identify and validate the specific vibrational modes that contribute strongly (or only weakly) to the reaction coordinate and has recently proved useful for investigating ultrafast molecular reaction dynamics [1]. We combine wave-packet-resolved femtosecond time-resolved fluorescence spectroscopy with molecular dynamics simulations to investigate the role of coherent nuclear motion and the quantum-mechanical nature of ultrafast photochemical reactions. Several examples of ultrafast coherent reaction dynamics will be presented. In particular, for an ultrafast excited-state proton-transfer reaction, we show that coherent nuclear motion plays a central role in determining the reaction pathway and timescale [2]. The results demonstrate that, in the ultrafast regime, reaction dynamics cannot be understood solely in terms of conventional energetic parameters such as reaction barriers and thermodynamic driving forces.

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