Laser-Controlled Nonadiabatic Processes in Excited-State Molecules

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Nonadiabatic processes in complex molecules either induced by interactions with laser light or part of transfer of electron excitation are present in many areas of physical, chemical und biological science. Modern experimental spectroscopic techniques, based on absorption, emission, pump-probe, or photodissociation processes, have already led to a wealth of information regarding the dynamics and reactivity on multiple excited electronic states. To interpret these experimental data, theoretical simulations of nonadiabatic dynamics need to be accurate and efficient. Many tools have been developed to theoretically study nonadiabatic molecular phenomena. Locating conical intersection with minimum energy provides topological information on the relevant potential energy surfaces and help to find the geometrical configurations that are crucial for understanding the movement or dynamics of atoms within a molecule. The goal of our research to investigate laser-induced nonadiabatic processes, in which a molecular wave function can controllably transition between states in two or more potential energy surfaces. Our control mechanism will rely on quantum interference of paths near conical intersections. Since electronically excited states are routinely formed when visible and higher-energy photons are absorbed, nonadiabatic processes are of fundamental importance in such areas as photosynthesis, solar energy conversion, and photochemistry.

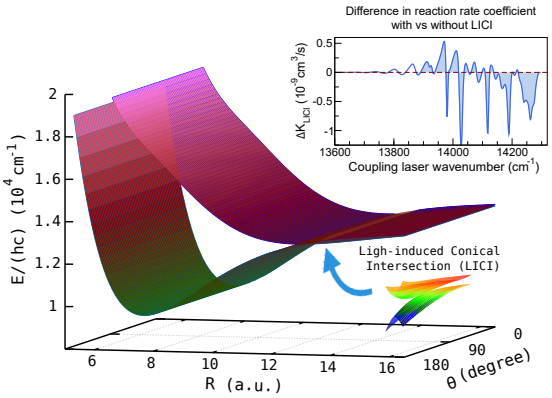

Figure 1: Difference between reaction rate coefficients with and without light-induced conical intersections