

Dynamics of Photoinduced Processes in the Diatomic Polar Molecules

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Quantum dynamics is a growing discipline at the interface of chemistry, physics, and materials science. It allows to study the behavior of objects in a way that emphasizes the quantum nature of their evolution in time. Quantum dynamics simulations are an indispensable tool for investigating processes such as chemical reactions, field-atoms interactions, and quantum computing. The particular emphasis is focused on investigating the photoinduced dynamics of breaking (dissociation) and creating (association) of the chemical bonds in the molecular systems. In the present work, we focus our attention on the theoretical time-dependent descriptions of the photoassociation and photodissociation processes in the polar alkali diatomic molecules. We investigate the photoinduced processes based on the high accuracy rovibrational and electronic structure of the polar alkali diatomic molecules, appropriate permanent and transition dipole moment functions (TDMF), and various types of coupling matrix elements, such for example nonadiabatic couplings or spin-orbit couplings. In the quantum simulations, we use our newly-developed quantum dynamics code that allows us to study the dynamics of multiple coupled states under the influence of an arbitrary time-dependent external field to investigate the femtosecond laser-driven processes like association and dissociation.