

Nonadiabatic Pathways of Photochemical Reactions

Hongmei Su

*Beijing National Laboratory for Molecular Sciences (BNLMS), State Key Laboratory of
Molecular Reaction Dynamics, Institute of Chemistry, Chinese Academy of Sciences, Beijing
100190, China*

E-mail: hongmei@iccas.ac.cn

Abstract

As known for the photochemistry of organic molecules, the reactive state is usually not the initially populated one. Ultrafast nonadiabatic transitions (IC or ISC) take place prior to the system reaching the reactive state, through which favorable nonadiabatic reaction pathways are open. We have explored the complicated nonadiabatic reaction pathways for several types of photochemical reactions including the photodissociation and photoisomerization of carbonyl compounds and the DNA photodamage reactions. The multiple electronic states participating the photochemical reactions are specified and the key roles played by surface intersections leading to the nonadiabatic reaction pathways are revealed.