



Advanced Series in Physical Chemistry - Vol. 17

CONICAL INTERSECTIONS

Theory, Computation and Experiment

edited by **Wolfgang Domcke** (Technical University of Munich, Germany), **David R Yarkony** (Johns Hopkins University, USA), & **Horst Köppel** (Heidelberg University, Germany)

The concept of adiabatic electronic potential-energy surfaces, defined by the Born–Oppenheimer approximation, is fundamental to our thinking about chemical processes. Recent computational as well as experimental studies have produced ample evidence that the so-called conical intersections of electronic energy surfaces, predicted by von Neumann and Wigner in 1929, are the rule rather than the exception in polyatomic molecules. It is nowadays increasingly recognized that conical intersections play a key mechanistic role in chemical reaction dynamics. This volume provides an up-to-date overview of the multi-faceted research on the role of conical intersections in photochemistry and photobiology, including basic theoretical concepts, novel computational strategies as well as innovative experiments. The contents and discussions will be of value to advanced students and researchers in photochemistry, molecular spectroscopy and related areas.

Contents: Fundamental Aspects and Electronic Structure: Conical Intersections in Organic Photochemistry (*M Robb*); Efficient Excited-State Deactivation in Organic Chromophores and Biologically Relevant Molecules: Role of Electron and Proton Transfer Processes (*A L Sobolewski & W Domcke*); Three-State Conical Intersections (*S Matsika*); Spin-Orbit Vibronic Coupling in Jahn-Teller Systems (*L V Poluyanov & W Domcke*); Symmetry Analysis of Geometric-Phase Effects in Quantum Dynamics (*S C Althorpe*); **Dynamics at Conical Intersections:** Conical Intersections in Electron Photodetachment Spectroscopy: Theory and Applications (*M S Schuurman & D R Yarkony*); Multi-State Vibronic Dynamics and Multiple

Conical Intersections (*S Faraji et al.*); Conical Intersections Coupled to an Environment (*I Burghardt et al.*); *Ab Initio* Multiple-Spawning: First-Principles Dynamics Around Conical Intersections (*S Yang & T J Martinez*); Non-Born-Oppenheimer Molecular Dynamics for Conical Intersections, Avoided Crossings and Weak Interactions (*A W Jasper & D G Truhlar*); Computational and Methodological Elements for Nonadiabatic Trajectory Dynamics Simulations of Molecules (*M Barbatti et al.*); Nonadiabatic Trajectory Calculations with *Ab Initio* and Semiempirical Methods (*E Fabiano et al.*); Multistate Nonadiabatic Dynamics “On the Fly” in Complex Systems and Its Control by Laser Fields (*R Mitric et al.*); Laser Control of Ultrafast Dynamics at Conical Intersections (*Y Ohtsuki & W Domcke*); **Experimental Detection of Dynamics at Conical Intersections:** Exploring Nuclear Motion Through Conical Intersections in the UV Photodissociation of Azoles, Phenols and Related Systems (*T A A Oliver et al.*); Interrogation of Nonadiabatic Molecular Dynamics via Time-Resolved Photoelectron Spectroscopy (*M S Schuurman & A Stolow*); Pump-Probe Spectroscopy of Ultrafast Vibronic Dynamics in Organic Chromophores (*F Renth et al.*); Femtosecond Pump-Probe Polarization Spectroscopy of Vibronic Dynamics at Conical Intersections and Funnels (*W K Peters et al.*).

Readership: Advanced students and researchers in photochemistry, molecular spectroscopy and related areas.

750pp	Aug 2011	
978-981-4313-44-5	US\$190	£131
978-981-4313-45-2(ebook)	US\$247	

