1. Record Nr. UNINA9910449877203321

| | |
|---|---|
| Titolo | Conical intersections [[electronic resource] ] : electronic structure, dynamics & spectroscopy / / editors : Wolfgang Domcke, David R. Yarkony, Horst Koppel |
| Pubbl/distr/stampa | River Edge, N. J. ; ; London, : World Scientific, 2004 |
| ISBN | 1-281-87701-8<br>9786611877019<br>981-256-546-9 |
| Edizione | [15th ed.] |
| Descrizione fisica | 1 online resource (857 p.) |
| Collana | Advanced series in physical chemistry ; ; v. 15 |
| Altri autori (Persone) | DomckeWolfgang<br>YarkonyDavid<br>KoppelHorst |
| Disciplina | 541.33 |
| Soggetti | Spectrum analysis<br>Laser spectroscopy<br>Molecular dynamics<br>Electronic books. |
| Lingua di pubblicazione | Inglese |
| Formato | Materiale a stampa |
| Livello bibliografico | Monografia |
| Note generali | Description based upon print version of record. |
| Nota di bibliografia | Includes bibliographical references and index. |
| Nota di contenuto | Introduction; Preface; Historical Introduction J. Michl; CONTENTS; 1. Born-Oppenheimer Approximation and Beyond L.S. Cederbaum; 2. Conical Intersections: Their Description and Consequences D.R. Yarkony; 3. Determination of Potential Energy Surface Intersections and Derivative Couplings in the Adiabatic Representation D.R. Yarkony; 4. Diabatic Representation: Methods for the Construction of Diabatic Electronic States H. Koppel; 5. Modeling and Interpolation of Global Multi-Sheeted Potential Energy Surfaces A.J.C. Varandas 6. Conical Intersections and Organic Reaction Mechanisms A. Migani and M. Olivucci7. The Multi-Mode Vibronic-Coupling Approach H. Koppel, W. Domcke and L.S. Cederbaum; 8. Model Studies of the Dynamics at Conical Intersections A. Lami and G. Villani; 9. Generic Aspects of the Dynamics at Conical Intersections: Internal Conversion, Vibrational Relaxation and Photoisomerization W. Domcke; 10. Jahn-Teller and Pseudo-Jahn-Teller Intersections: Spectroscopy and Vibronic |

Dynamics H. Koppel

11. Quantum Mechanical Studies of Photodissociation Dynamics Using Accurate Global Potential Energy Surfaces R. Schinke12. Geometric Phase Effects in Chemical Reaction Dynamics B.K. Kendrick; 13. Quantum Reaction Dynamics on Coupled Multi-Sheeted Potential Energy Surfaces S. Mahapatra; 14. Multidimensional Dynamics Involving a Conical Intersection: Wavepacket Calculations Using the MCTDH Method G.A. Worth, H.-D. Meyer and L.S. Cederbaum; 15. Mixed Quantum-Classical Description of the Dynamics at Conical Intersections G. Stock and M. Thoss

16. Absorption, Emission, and Photoelectron Continuous-Wave Spectra A. Lami, C. Petrongolo and F. Santoro17. Femtosecond Time-Resolved Spectroscopy of the Dynamics at Conical Intersections G. Stock and W. Domcke; 18. Nonadiabatic Quantum Dynamics and Control Strategies R. de Vivie-Riedle and A. Hofmann; Index

Sommario/riassunto

It is widely recognized nowadays that conical intersections ofmolecular potential-energy surfaces play a key mechanistic role in thespectroscopy of polyatomic molecules, photochemistry and chemicalkinetics. This invaluable book presents a systematic exposition of thecurrent state of knowledge about conical intersections, which has beenelaborated in research papers scattered throughout the chemicalphysics literature.