

| | |
|-------------------------|---|
| 1. Record Nr. | UNINA9910809396703321 |
| Titolo | Conical intersections : 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 9786611877019 981-256-546-9 |
| Edizione | [15th ed.] |
| Descrizione fisica | 1 online resource (857 p.) |
| Collana | Advanced series in physical chemistry ; ; v. 15 |
| Classificazione | 35.10 |
| Altri autori (Persone) | DomckeWolfgang YarkonyDavid KoppelHorst |
| Disciplina | 541.33 |
| Soggetti | Spectrum analysis Laser spectroscopy Molecular dynamics |
| 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. Schinke
12. 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. Santoro
17. 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 of molecular potential-energy surfaces play a key mechanistic role in the spectroscopy of polyatomic molecules, photochemistry and chemical kinetics. This invaluable book presents a systematic exposition of the current state of knowledge about conical intersections, which has been elaborated in research papers scattered throughout the chemical physics literature.
