

1. Record Nr.	UNINA9910139033003321
Titolo	Advances in chemical physics [[electronic resource]] . Volume 153 // edited by Stuart A. Rice, Aaron R. Dinner
Pubbl/distr/stampa	Hoboken, N.J., : Wiley, 2013
ISBN	1-118-57176-2 1-118-57175-4 1-299-40239-9 1-118-57180-0
Edizione	[2nd ed.]
Descrizione fisica	1 online resource (599 p.)
Collana	Advances in chemical physics ; ; v. 153
Altri autori (Persone)	RiceStuart A DinnerAaron R
Disciplina	535.2 539
Soggetti	Chemistry, Physical and theoretical
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 indexes.
Nota di contenuto	Advances In Chemical Physics; Contributors; Preface to The Series; Contents; Recent Advances in Ultrafast X-ray Absorption Spectroscopy of Solutions; I. Introduction; II. Experimental Methods; A. Steady-State XAS; 1. Transmission and Fluorescence Detection Modes; B. Time-Resolved XAS; 1. General Setup; 2. Interpretation of the Transient Signal; C. Sources of Ultrafast X-ray Pulses and Data Acquisition; 1. Picosecond XAS; 2. Femtosecond XAS: The Slicing Scheme; 3. Future Developments: X-FELs; III. Theoretical Approaches for XAFS; A. Structural Analysis: The EXAFS Region B. The Quasiparticle Approximation: Modeling the Near Edge 1. Green's Functions and Multiple Scattering Theory; 2. Beyond Spherical Potentials; C. Many-Body Effects; 1. The Self-Energy Operator; 2. Time-Dependent Density Functional Theory; 3. Post-Hartree-Fock Methods; D. Beyond Picosecond Temporal Resolution; IV. Examples; A. Photoinduced Hydrophobicity; B. Spin-Crossover Molecular Systems; C. Solvent Effects; D. Intramolecular Charge Transfer; V. Outlook; Acknowledgments; References; Scaling Perspective on Intramolecular Vibrational Energy Flow: Analogies, Insights, and Challenges

I. Introduction: Motivation and Historical Overview II. IVR: Analogy to Anderson Localization; A. Introducing the IVR State Space; B. Quantum Ergodicity Threshold; 1. Ensemble of Hamiltonians: Probabilistic Approach to the Transition; III. Scaling Theory of IVR; A. State Space Predictions; IV. Important Questions; V. Classical-Quantum Correspondence and IVR; A. State Space-Phase Space Correspondence; B. Geometry of the Resonance Network: Arnold Web; C. Computing the Arnold Web; 1. Variational Approaches; 2. Time-Frequency Analysis; 3. "Coarse-Grained" Frequency Ratio Space
5. Kramers' Formula as a Special Case of Langer's Formula B. Kramers' Turnover Problem; 1. Green Function of the Energy-Action Diffusion Equation; 2. Integral Equation for the Distribution Function in Energy-Action Variables; 3. Kramers' VLD Result; 4. Criticisms of the Ad Hoc Approach of Mel'nikov and Meshkov; C. Applications of the Theory of Brownian Movement in a Potential and of the Kramers Theory; D. Escape Rate for a Fixed Axis Rotator in a Double-Well Potential; 1. Turnover Formula for the Escape Rate for Fixed Axis Rotation
2. Exact Matrix Continued Fraction Solution of the Langevin Equation

Sommario/riassunto

Detailed reviews of new and emerging topics in chemical physics presented by leading experts The Advances in Chemical Physics series is dedicated to reviewing new and emerging topics as well as the latest developments in traditional areas of study in the field of chemical physics. Each volume features detailed comprehensive analyses coupled with individual points of view that integrate the many disciplines of science that are needed for a full understanding of chemical physics. Volume 153 of Advances in Chemical Physics features six expertly written
