1. Record Nr. UNINA9910824926003321

Autore	Scott K (Keith), <1951->
Titolo	Sustainable and green electrochemical science and technology / / Keith Scott
Pubbl/distr/stampa	Hoboken, New Jersey : , : Wiley Blackwell, , 2017 ©2017
ISBN	1-118-69810-X 1-118-69808-8 1-118-69807-X
Descrizione fisica	1 online resource (411 pages)
Disciplina	541/.37
Soggetti	Electrochemistry Green electronics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di bibliografia	Includes bibliographical references and index.

2. Record Nr. UNINA9910818938103321

Titolo	Modeling of molecular properties / / edited by Peter Comba
Pubbl/distr/stampa	Weinheim, : Wiley-VCH, c2011
ISBN	9783527636419 3527636412 9781283869775 1283869772 9783527636426 3527636420 9783527636402 3527636404
Edizione	[2nd ed.]
Descrizione fisica	1 online resource (513 p.)
Altri autori (Persone)	CombaPeter
Disciplina	541.220113 620.11299
Soggetti	Biochemistry Chemistry, Inorganic Chemistry, Organic Molecules - Models
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	Modeling of Molecular Properties; Contents; Preface; List of Contributors; Part One: Theory and Concepts; 1 Accurate Dispersion-Corrected Density Functionals for General Chemistry Applications; 1.1 Introduction; 1.2 Theoretical Background; 1.2.1 Double-Hybrid Density Functionals; 1.2.2 London-Dispersion-Corrected DFT; 1.3 Examples; 1.3.1 GMTKN30; 1.3.2 A Mechanistic Study with B2PLYP-D; 1.3.3 Double-Hybrids for Excited States; 1.4 Summary and Conclusions; References; 2 Free-Energy Surfaces and Chemical Reaction Mechanisms and Kinetics; 2.1 Introduction; 2.2 Elementary Reactions 2.3 Two Consecutive Steps2.4 Multiple Consecutive Steps; 2.5 Competing Reactions; 2.6 Catalysis; 2.7 Conclusions; References; 3 The Art of Choosing the Right Quantum Chemical Excited-State Method for

Large Molecular Systems; 3.1 Introduction; 3.2 Existing Excited-State Methods for Medium-Sized and Large Molecules; 3.2.1 Wavefunction-Based ab initio Methods; 3.2.2 Density-Based Methods; 3.3 Analysis of Electronic Transitions; 3.4 Calculation of Static Absorption and Fluorescence Spectra; 3.5 Dark States; 3.5.1 Excited Electronic States with Large Double Excitation Character
3.5.2 Charge-Transfer Excited States3.6 Summary and Conclusions; References; 4 Assigning and Understanding NMR Shifts of Paramagnetic Metal Complexes; 4.1 The Aim and Scope of the Chapter; 4.2 Basic Theory of Paramagnetic NMR; 4.2.1 The Origin of the Hyper.ne Shift; 4.2.1.1 The Contact Shift; 4.2.1.2 The Pseudocontact Shift; 4.2.2 Relaxation and Line Widths; 4.2.2.1 Electronic Relaxation; 4.2.2.2 Dipolar Relaxation; 4.2.2.3 Contact Relaxation; 4.2.2.4 Curie Relaxation; 4.2.3 Advice for Recording Paramagnetic NMR Spectra; 4.3 Signal Assignments; 4.3.1 Comparison of Similar Compounds
4.3.2 Separation of Contact and Pseudocontact Shift4.3.3 Estimating the Dipolar Contributions; 4.3.4 DFT-Calculation of Spin-Densities; 4.4 Case Studies; 4.4.1 Organochromium Complexes; 4.4.2 Nickel Complexes; References; 5 Tracing Ultrafast Electron Dynamics by Modern Propagator Approaches; 5.1 Charge Migration Processes; 5.1.1 Theoretical Considerations of Charge Migration; 5.2 Interatomic Coulombic Decay in Noble Gas Clusters; 5.2.1 Theoretical Considerations of ICD; References; 6 Natural Bond Orbitals and Lewis-Like Structures of Copper Blue Proteins
6.1 Introduction: Localized Bonding Concepts in Copper Chemistry6.2 Localized Bonds and Molecular Geometries in Polyatomic Cu Complexes; 6.3 Copper Blue Proteins and Localized Bonds; 6.4 Summary; References; 7 Predictive Modeling of Molecular Properties: Can We Go Beyond Interpretation?; 7.1 Introduction; 7.2 Models and Modeling; 7.3 Parameterized Classical and Quantum Mechanical Theories; 7.4 Predictive Energies and Structures; 7.5 Other Gas-Phase Properties; 7.6 Solvent Effects: The Major Problem; 7.7 Reaction Selectivity; 7.8 Biological and Pharmaceutical Modeling; 7.8.1 SAR Modeling
7.8.2 Force Fields, Docking, and Scoring

Sommario/riassunto

Molecular modeling encompasses applied theoretical approaches and computational techniques to model structures and properties of molecular compounds and materials in order to predict and / or interpret their properties. The modeling covered in this book ranges from methods for small chemical to large biological molecules and materials. With its comprehensive coverage of important research fields in molecular and materials science, this is a must-have for all organic, inorganic and biochemists as well as materials scientists interested in applied theoretical and computational chemistry. The 28