1. Record Nr. UNICAMPANIASUN0090157

Titolo	Il palazzo della Ragione di Padova : la storia, l'architettura, il restauro / a cura di Ettore Vio
Pubbl/distr/stampa	Padova : Signumpadova, 2004
ISBN	978-88-8475-021-1
Descrizione fisica	391 p., 9 c. di tav. : ill. ; 30 cm.
Lingua di pubblicazione	Italiano
Formato	Materiale a stampa
Livello bibliografico	Monografia

2. Record Nr. UNINA9911019420803321

Autore	Liu Shubin
Titolo	Exploring Chemical Concepts Through Theory and Computation
Pubbl/distr/stampa	Newark : , : John Wiley & Sons, Incorporated, , 2024 ©2024
ISBN	9783527843411 3527843418 9783527843435 3527843434 9783527843428 3527843426
Edizione	[1st ed.]
Descrizione fisica	1 online resource (594 pages)
Disciplina	542.8
Soggetti	Computational chemistry Quantum chemistry
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Cover -- Title Page -- Copyright -- Contents -- Preface -- Foreword

-- Chapter 12 On the Generalization of Marcus Theory for TwoState Photophysical Processes -- 12.1 Introduction -- 12.2 The Golden Rule Rate Expression -- 12.2.1 The Marcus Theory: The Classical Treatment -- 12.2.2 The Marcus-Levich-Jortner Expression: A Quantum Expression for HighFrequency Modes -- 12.2.3 The Föster Theory: Separating Donor and Acceptor Parts in FCWD -- 12.3 Application -- 12.3.1 Electron Transfer -- 12.3.2 SET: Using Spectra for FCWD -- 12.3.3 TET and Other Energy Transfer Process with Spin Exchange -- 12.4 Conclusion -- Acknowledgments -- References -- Chapter 13 Computational Modeling of CO2 Reduction and Conversion via Heterogeneous and Homogeneous Catalysis -- 13.1 Introduction -- 13.2 Computational Methods -- 13.3 Activation and Reduction of CO2 -- 13.3.1 Computational Catalyst Design -- 13.3.1.1 Doping of Metal and Nonmetal Atoms -- 13.3.1.2 Structural Modification -- 13.3.1.3 Application of an External Electric Field -- 13.3.2 Electrocatalytic Reduction of CO2 -- 13.3.3 Hydrogenation Reduction of CO2 -- 13.4 Catalytic Coupling of CO2 with CH4 -- 13.5 Homogeneous Catalytic Conversion of CO2 -- 13.5.1 Catalytic CO2 Fixation into Cyclic Carbonates -- 13.5.2 CO2 Hydrogenation Catalyzed by Metal PNP Pincer Complexes -- 13.6 Conclusion and Outlook -- Acknowledgments -- References -- Chapter 14 Excited States in Conceptual DFT -- 14.1 Introduction -- 14.2 Exploring Ground State Properties Thanks to Excited States -- 14.2.1 Context and Justification -- 14.2.2 Chemical Hardness Revisited -- 14.2.3 StateSpecific Dual Descriptors -- 14.2.4 Polarization Interaction -- 14.3 Exploring the Reactivity of Excited States with Excited States.
14.3.1 Local Chemical Potential.

Sommario/riassunto

This comprehensive book, edited by Shubin Liu, delves into the exploration of chemical concepts through theoretical and computational chemistry. It covers a broad range of topics including molecular orbital theory, valence bond theory, density functional theory, and energy decomposition analysis. The book aims to provide insights into chemical bonding, partial charges, aromaticity, and various other fundamental chemical concepts. The chapters are contributed by numerous experts, offering both static and dynamic properties of chemical entities. This resource is invaluable for researchers, academics, and advanced students in the field of chemistry who are interested in understanding the theoretical underpinnings and computational approaches that define chemical principles and empirical laws.