1. Record Nr. UNINA9910828691603321

Titolo	Computational chemistry : reviews of current trends. Vol. 9 / / editor, Jerzy Leszczynski
Pubbl/distr/stampa	Hackensack, N.J., : World Scientific, 2005
ISBN	1-281-89704-3 9786611897048 981-270-130-3
Edizione	[1st ed.]
Descrizione fisica	1 online resource (258 p.)
Altri autori (Persone)	LeszczynskiJerzy <1949->
Disciplina	542.85
Soggetti	Chemistry - Mathematics
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	PREFACE; CONTENTS; Chapter 1: Molecular Electronics with Gaussian98/03; Chapter 2: Molecular Dynamics Simulations of Single Molecule Atomic Force Microscope Experiments; Chapter 3: Molecular Dynamics Simulations of a Molecular Electronics Device: The NanoCell; Chapter 4: Computation of Excited State Potential Energy Surfaces via Linear Response Theories Based on State Specific Multi-Reference Coupled Electron-Pair Approximation Like Methods Chapter 5: Modelling of Anisotropic Exchange Coupling in Rare-Earth - Transition-Metal Pairs: Applications to Yb3+-Mn2+ and Yb3+-Cr3+ Halide Clusters and Implications to the Light Up-ConversionChapter 6: Is a Dihydrogen Bond a Unique Phenomenon?; INDEX; CONTENT INDEX
Sommario/riassunto	Vast progress in the area of computational chemistry has been achieved in the last decade. Theoretical methods such as quantum mechanics, molecular dynamics and statistical mechanics have been successfully used to characterize chemical systems and to design new materials, drugs and chemicals. The reviews presented in this volume discuss the current advances in computational methodologies and their applications. The areas covered include materials science, nanotechnology, inorganic and biological systems. The major thrust of the book is to bring timely overviews of new findings and methods appl