Record Nr. UNINA9910451347603321 Computational chemistry [[electronic resource]]: reviews of current **Titolo** 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 Descrizione fisica 1 online resource (258 p.) Altri autori (Persone) LeszczynskiJerzy <1949-> Disciplina 542.85 Chemistry - Mathematics Soggetti Electronic books. 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 Gaussian 98/03; 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 Vast progress in the area of computational chemistry has been Sommario/riassunto 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