

1. Record Nr.	UNINA9910566465403321
Autore	Altaf-UI-Amin Md
Titolo	Recent Trends in Computational Research on Diseases
Pubbl/distr/stampa	Basel, : MDPI - Multidisciplinary Digital Publishing Institute, 2022
Descrizione fisica	1 online resource (130 p.)
Soggetti	History of engineering & technology Technology: general issues
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Sommario/riassunto	<p>Recent advances in information technology have brought forth a paradigm shift in science, especially in the biology and medical fields. Statistical methodologies based on high-performance computing and big data analysis are now indispensable for the qualitative and quantitative understanding of experimental results. In fact, the last few decades have witnessed drastic improvements in high-throughput experiments in health science, for example, mass spectrometry, DNA microarray, next generation sequencing, etc. Those methods have been providing massive data involving four major branches of omics (genomics, transcriptomics, proteomics, and metabolomics). Information about amino acid sequences, protein structures, and molecular structures are fundamental data for the prediction of bioactivity of chemical compounds when screening drugs. On the other hand, cell imaging, clinical imaging, and personal healthcare devices are also providing important data concerning the human body and disease. In parallel, various methods of mathematical modelling such as machine learning have developed rapidly. All of these types of data can be utilized in computational approaches to understand disease mechanisms, diagnosis, prognosis, drug discovery, drug repositioning, disease biomarkers, driver mutations, copy number variations, disease pathways, and much more. In this Special Issue, we have published 8 excellent papers dedicated to a variety of computational problems in</p>

the biomedical field from the genomic level to the whole-person physiological level.

2. Record Nr.	UNINA9910865272903321
Autore	Grabowski Ireneusz
Titolo	Advances in Methods and Applications of Quantum Systems in Chemistry, Physics, and Biology : Selected Proceedings of QSCP-XXV Conference (Toru, Poland, June 2022) // edited by Ireneusz Grabowski, Karolina Sowik, Jean Maruani, Erkki J. Brändas
Pubbl/distr/stampa	Cham : , : Springer Nature Switzerland : , : Imprint : Springer, , 2024
ISBN	3-031-52078-5
Edizione	[1st ed. 2024.]
Descrizione fisica	1 online resource (300 pages)
Collana	Progress in Theoretical Chemistry and Physics, , 2215-0129 ; ; 34
Altri autori (Persone)	SowikKarolina MaruaniJean BrändasErkki J
Disciplina	530.12
Soggetti	Chemistry, Physical and theoretical Chemistry - Data processing Quantum chemistry Atoms Molecules Molecular dynamics Theoretical Chemistry Computational Chemistry Quantum Chemistry Atomic, Molecular and Chemical Physics Molecular Dynamics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Part I. General Theory -- Landauer's Principle and Thermodynamics -- On the Majorana Solution to the Thomas-Fermi Equation -- Spherically Averaged Densities as Basic DFT Variables -- Linear-Expansion Shooting Techniques Based on Minimization of Intra-Iteration Errors --

Part II. Atomic Systems -- Erfonium: A Hooke Atom with Soft Interaction Potential -- Spectroscopy of Radiative Decay Processes in Atomic Systems in a Black-body Radiation Field -- Relativistic Many-Body Perturbation Theory Approach to Computing Spectra of Complex Atomic Systems: Spectral Data for Ne-like Ions -- Relativistic Quantum Chemistry and Spectroscopy of Pionic Atomic Systems: Hyperfine Structure -- Part III. Molecular Systems -- Low-Cost Generation of Optimal Molecular Orbitals for Multi-Reference CI Expansion: Natural Orbitals versus Renyi Entropy-Minimized Orbitals Provided by the Density-Matrix Renormalization Group -- Formally Exact Many-Body Perturbation Theory with Optimized Zeroth Approximation in Calculations of Spectral Parameters of Diatomic Molecules -- Complexes of Counterion-Trapped Molecules: Extreme Polarity, Rich IR-Activity, and Internal-Field Moderated Transformations -- Designing an Iron-Based Bis(pyridyl)borate Complex Catalyst for Ammonia-Borane Dehydrogenation using Density Functional Theory -- Theoretical Investigation of Cl₂, ClO and Cl₂O Molecules -- Part IV. Biochemistry and Biophysics -- An Improved Fragmentation Modeling Aminoacids Under Ionizing Radiation. I. Threonine -- Computational Investigation of the Influence of the Acyl Group on the Reducing Abilities of Acylphloroglucinols -- Integrated in-Silico Drug Modeling for Viral Proteins.

Sommario/riassunto

This book contains peer-reviewed contributions based on talks presented at the 25th International Workshop on Quantum Systems in Chemistry, Physics, and Biology held in Toru, Poland, in June 2022. The book reviews significant advances in concepts, methods, and applications of quantum systems in a broad variety of areas in modern chemistry, physics, and biology. In particular, it discusses atomic, molecular, and solid state structure, dynamics and spectroscopy, relativistic and correlation effects in quantum chemistry, topics of computational chemistry, physics, and biology, as well as applications of theoretical chemistry and physics in advanced molecular and nano-materials and biochemical systems. This book is aimed at advanced graduate students, academics, and researchers, both in university and corporation laboratories, interested in state of the art and novel trends in quantum chemistry, physics, and biology, and their applications. .
