

1. Record Nr.	UNINA9910380724803321
Titolo	Advances in Quantum Systems in Chemistry, Physics, and Biology : Selected Proceedings of QSCP-XXIII (Kruger Park, South Africa, September 2018) // edited by Liliana Mammino, Davide Ceresoli, Jean Maruani, Erkki Brändas
Pubbl/distr/stampa	Cham : , : Springer International Publishing : , : Imprint : Springer, , 2020
ISBN	3-030-34941-1
Edizione	[1st ed. 2020.]
Descrizione fisica	1 online resource (XVI, 469 p.)
Collana	Progress in Theoretical Chemistry and Physics, , 1567-7354 ; ; 32
Disciplina	541.28
Soggetti	Chemistry, Physical and theoretical Atomic structure Molecular structure Bioinformatics Computational biology Quantum physics Theoretical and Computational Chemistry Atomic/Molecular Structure and Spectra Computer Appl. in Life Sciences Quantum Physics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Includes index.
Nota di contenuto	Part 1: Exotic Atomic Systems -- Chapter 1. Advanced Relativistic Energy Approach in the Spectroscopy of Auto-ionization States of Multi-electron Atomic Systems (Alexander V. Glushkov) -- Chapter 2. Relativistic Quantum Chemistry and Spectroscopy of Kaonic Atomic Systems with Accounting for Radiative and Strong Interaction Effects(O. Yu. Khetselius, V. B. Ternovsky, Y.V. Dubrovskaya, I.N. Serga,and A. A. Svinarenko) -- Chapter 3. Spectroscopy of Rydberg Atomic Systems in a Black-Body Radiation Field (Valentin B. Ternovsky, Alexander V. Glushkov, Anna A. Kuznetsova, and Andrey V. Tsudik) -- Chapter 4. Hyperfine and Electroweak Interactions in Heavy Finite Fermi Systems and Parity Non-conservation Effect(Olga Yu. Khetselius, Alexander V.

Glushkov, Eugeny Ternovsky, Vasily V. Buyadzi, and Aleksii L. Mykhailov) -- Part 2: Clusters and Molecules Interactions -- Chapter 5. Quantum Study of Helium Clusters Doped with Electronically Excited Li, Na, K and Rb Atoms (David Dell'Angelo). -- Chapter 6. A Quantum Chemical Approach for the Characterization of the Interaction Potential of Propylene Oxide with Rare-Gas Atoms (He, Ne, Ar)(Partricia R. P. Barreto, Ana Claudia P. S. Cruz, Henrique O. Euclides, Alessandra F. Albernaz, Federico Palazzetti, and Fernando Pirani) -- Chapter 7. A Theoretical Study on the Reaction between Chloroacetic Acid and Thiourea(Mwadham M. Kabanda and Kgalaletso P. Otukile) -- Chapter 8. Density Functional Theory Studies of Ruthenium (N3) Dye Adsorbed on a TiO₂ Brookite Nanocluster for Application to Dye Sensitized Solar Cells (I. F. Elegbeleye, N. E. Maluta, and R. R. Maphanga) -- Part 3: Biochemistry and Biophysics -- Chapter 9. Complexes of Furonequinone-B with a Cu²⁺ Ion. A DFT Study (Liliana Mammino) -- Chapter 10. Computational Study of Shuangancistroretorine-A: A Naphthyliso-quinoline Alkaloid with Antimalarial Activity(Mireille Bilonda and Liliana Mammino) -- Chapter 11. Ab initio and DFT Computational Study of Myristinin-A and a Structurally Related Molecule(Neani Tshilande and Liliana Mammino) -- Chapter 12. Current Problems in Computer Simulation of Variability of the Three-Dimensional Structure of DNA(V. Poltev, V.M. Anisimov1, V. Dominguez, A. Deriabina, E. Gonzalez, D. Garcia, V. Vázquez-Báez, F. Rivas) -- Part 4: Fundamental Theory -- Chapter 13. Efficient 'Middle' Thermostat Scheme for the Quantum / Classical Canonical Ensemble via Molecular Dynamics (Xinzijian Liu, Kangyu Yan, and Jian Liu) -- Chapter 14. Megascopic Quantum Phenomena: A Critical Study of Physical Interpretations (Michal Crvek) -- Chapter 15. Is Abiogenesis Supported by the Second Law of Thermodynamics? (Erkki J. Brändas) -- Chapter 16. Can Quantum Theory Concepts Shed Light on Biological Evolution Processes? (Jean Maruani).

Sommario/riassunto

This edited, multi-author book gathers selected, peer-reviewed contributions based on papers presented at the 23rd International Workshop on Quantum Systems in Chemistry, Physics, and Biology (QSCP-XXIII), held in Mopani Camp, The Kruger National Park, South Africa, in September 2018. The content is primarily intended for scholars, researchers, and graduate students working at universities and scientific institutes who are interested in the structure, properties, dynamics, and spectroscopy of atoms, molecules, biological systems, and condensed matter.
