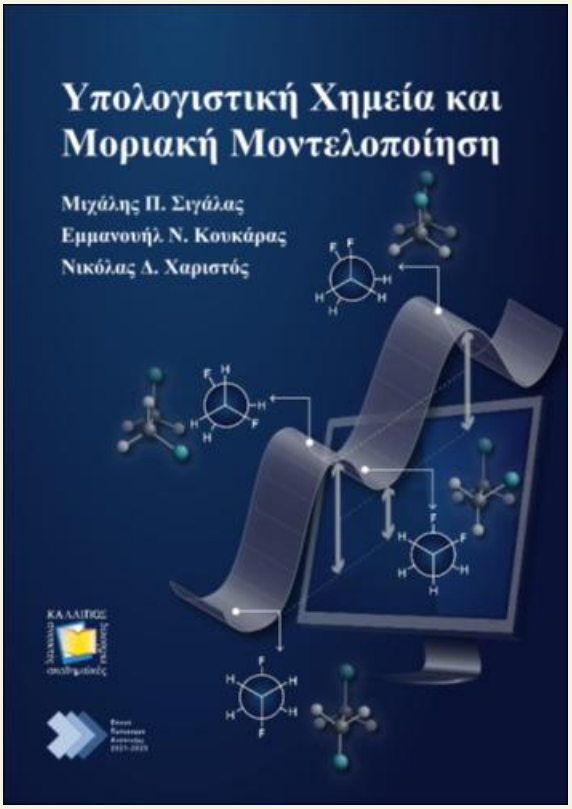

METADATA

Title: Computational Chemistry and Molecular Modeling

Other Titles: -

Language: Greek

Authors: Sigalas, M., Professor, AUTH, Koukaras, E., Professor, AUTH, Charistos, N., Professor AUTH

ISBN: 978-618-228-278-6

Subject: NATURAL SCIENCES AND AGRICULTURAL SCIENCES

Keywords: Computational Chemistry / Molecular Modeling / Quantum Chemistry / Molecular Mechanics / Molecular Dynamics

Bibliographic Reference: Sigalas, M., Koukaras, E., & Charistos, N. (2024). Computational Chemistry and Molecular Modeling [Undergraduate textbook]. Kallipos, Open Academic Editions. http://dx.doi.org/10.57713/kallipos-1024

Abstract

The fields of Computational Chemistry and Molecular Modeling involve the development and application of computational methods for studying molecular structure and physicochemical and spectroscopic properties of chemical systems. The methods fall into two distinct scientific fields, Quantum Chemistry, which applies Quantum Mechanics to chemical systems, and Molecular Mechanics/Dynamics, which apply Classical and Analytical Mechanics and Statistical Physics. Through dialectical handling of the topics, the book strives to cultivate in readers a critical understanding of the significance and limitations of the different computational models. In quantum chemical computational models, theories such as Hartree–Fock, Møller–Plesset perturbation theory, configuration interaction theory, coupled cluster theory, and density functional theory are presented. In classical computational models, force fields and the dynamics of chemical systems through Molecular Dynamics are presented and analysed. General computational techniques, such as partial or full geometry optimisations, scanning of potential energy surface, and vibrational analysis, are introduced. The book provides combined knowledge, covering both fundamental theoretical frameworks and practical applications in computational analysis, aiming to enable readers to conduct independent research and analysis in their field. The theoretical development of the topics is complemented by examples and applications using well-known scientific software, allowing students to apply theoretical knowledge to practical problems. This book serves as an introduction to the theoretical principles and application methodologies of the aforementioned computational models. It is primarily addressed to students of Chemistry, Material Science, Chemical Engineering, and Physics departments. These subjects are taught either as standalone courses or partially integrated into other courses such as Theoretical and Quantum Chemistry, Molecular Physics, Applied Quantum Mechanics, Inorganic and Organic Chemistry, and Spectroscopy.

The Project is funded by the National Development Programme 2021-2025 of the Ministry of Education and Religious Affairs and implemented by the Special Account for Research Funds of the National Technical University of Athens and the Hellenic Academic Libraries Link.