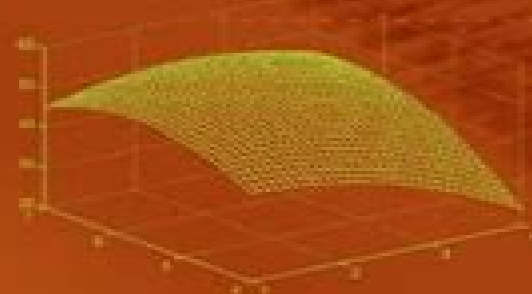


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Computational Chemistry and Molecular Modeling

Principles and
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Mario Leclerc, Robert Gauvin



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Molecular Modeling Hans-Dieter Höltje, Gerd Folkers, 2008-07-11. Written by experienced experts in molecular modeling, this book describes the basics to the extent that is necessary if one wants to be able to reliably judge the results from molecular modeling calculations. Its main objective is the description of the various pitfalls to be avoided. Without unnecessary overhead, it leads the reader from simple calculations on small molecules to the modeling of proteins and other relevant biomolecules. A textbook for beginners as well as an invaluable reference for all those dealing with molecular modeling in their daily work.

Computational Studies Ambrish Kumar Srivastava, 2024-08-06. The book covers a diverse range of topics based on computational studies including modeling and simulations based on quantum chemical studies and molecular dynamics MD simulations. It contains quantum chemical studies on several molecules including biologically relevant molecules and liquid crystals and various aspects of superatomic clusters including superalkalis and superhalogens. It gives an overview of MD simulations and their applications on biomolecular systems such as HIV 1 protease and integrase. Features: Includes first principle methods, density functional theory, as well as molecular dynamics simulations. Explores quantum chemical studies on several molecules. Gives readers an overview of the power of computation. Discusses superatomic clusters, superalkalis, and superhalogens. Covers themes from molecules, clusters, materials, as well as biophysical systems. This book is aimed at researchers and graduate students in materials science and computational and theoretical chemistry.

Functional Materials Mario Leclerc, Robert Gauvin, 2014-10-10. Functional Materials textbook is not simply a review of the vast body of literature of the recent years as it holds the focus upon various aspects of application. Moreover, it selects only a few topics in favor of a solid and thorough treatment of the relevant aspects. This book comes in a good time when a large body of academic literature has been accumulated and is waiting for a critical inspection in the light of the real demands of application. Professor Gerhard Wegner, Max Planck Institute for Polymer Research, Mainz, Germany. The chapters cover three

important fields in the development of functional materials energy environment and biomedical applications These topics are explained and discussed from both an experimental and a theoretical perspective Functional organic and inorganic materials are at the center of most technological breakthroughs Therefore the understanding of material properties is fundamental to the development of novel functionalities and applications

Kinetics and Dynamics Piotr Paneth, Agnieszka

Dybala-Defratyka, 2010-08-03 Kinetics and Dynamics on molecular modeling of dynamic processes opens with an introductory overview before discussing approaches to reactivity of small systems in the gas phase Then it examines studies of systems of increasing complexity up to the dynamics of DNA This title has interdisciplinary character presenting wherever possible an interplay between the theory and the experiment It provides basic information as well as the details of theory and examples of its application to experimentalists and theoreticians interested in modeling of dynamic processes in chemical and biochemical systems All contributing authors are renowned experts in their fields and topics covered in this volume represent the forefront of today's science

Computational Chemistry David Young, 2004-04-07

A practical easily accessible guide for bench top chemists this book focuses on accurately applying computational chemistry techniques to everyday chemistry problems Provides nonmathematical explanations of advanced topics in computational chemistry Focuses on when and how to apply different computational techniques Addresses computational chemistry connections to biochemical systems and polymers Provides a prioritized list of methods for attacking difficult computational chemistry problems and compares advantages and disadvantages of various approximation techniques Describes how the choice of methods of software affects requirements for computer memory and processing time

Hybrid Methods of Molecular Modeling Andrei L.

Tchougréeff, 2008-08-01 Hybrid Methods of Molecular Modeling is a self contained advanced review offering step by step derivation of the consistent theoretical picture of hybrid modeling methods and the thorough analysis of the concepts and current practical methods of hybrid modeling based on this theory Hybrid Methods of Molecular Modeling presents its material in a sequential way paying attention both to the physical soundness of the approximations used and to the mathematical rigor necessary for practical developing of the robust modeling code Historical remarks are given when it is necessary to put the current presentation in a more general context and to establish relation with other areas of computational chemistry The reader should have experience with basic concepts of computational chemistry and or molecular modeling Basic knowledge of operators wave functions electron densities is necessary

Quantum Modeling of

Complex Molecular Systems Jean-Louis Rivail, Manuel Ruiz-Lopez, Xavier Assfeld, 2015-10-13 This multi author contributed volume includes methodological advances and original applications to actual chemical or biochemical phenomena which were not possible before the increased sophistication of modern computers The chapters contain detailed reviews of the developments of various computational techniques used to study complex molecular systems such as molecular liquids and solutions particularly aqueous solutions liquid gas solid gas interphase and biomacromolecular systems Quantum modeling of

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