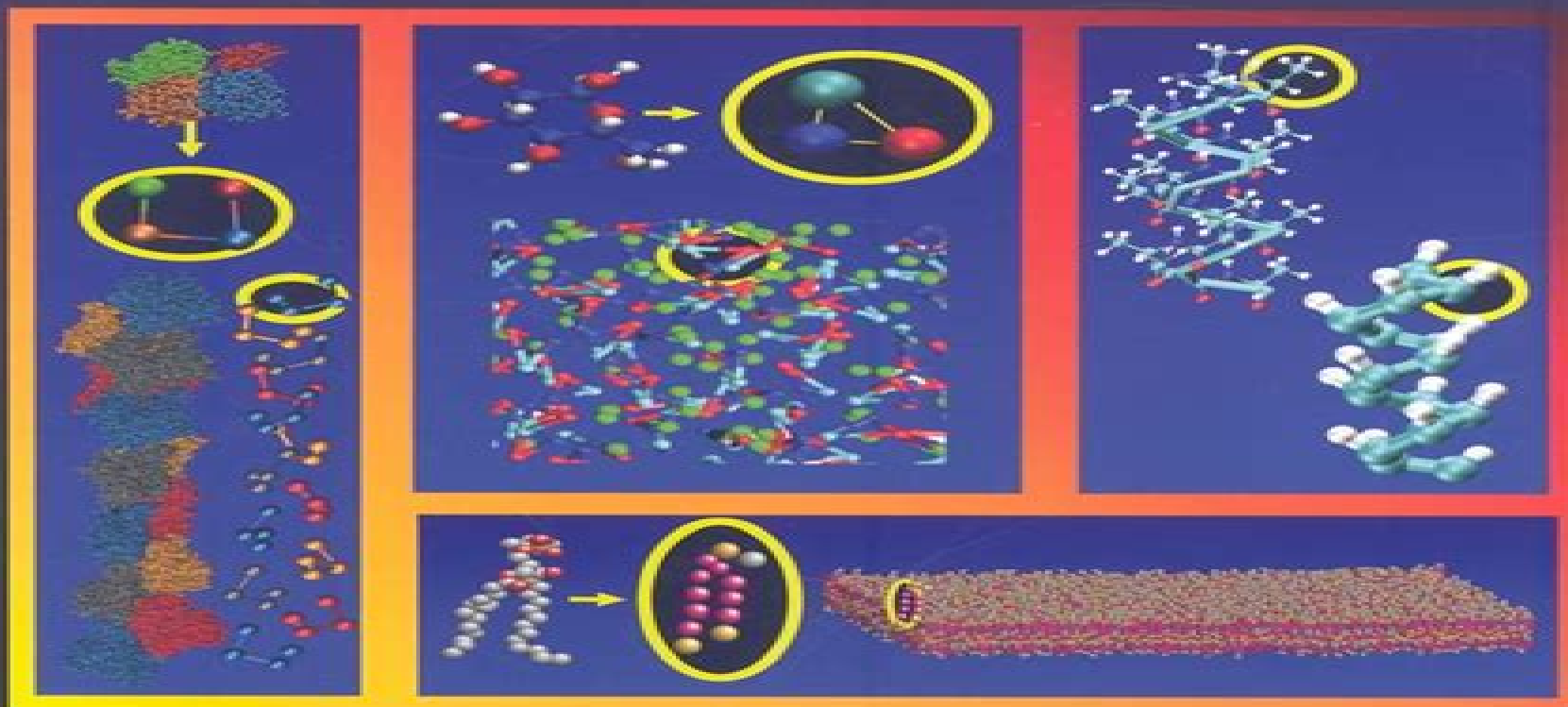


Coarse-Graining of Condensed Phase and Biomolecular Systems



Edited by
Gregory A. Voth



CRC Press
Taylor & Francis Group

Coarse Graining Of Condensed Phase And Biomolecular Systems

Robert R. Redfield



Coarse Graining Of Condensed Phase And Biomolecular Systems:

Coarse-Graining of Condensed Phase and Biomolecular Systems Gregory A. Voth, 2008-09-22 Exploring recent developments in the field Coarse Graining of Condensed Phase and Biomolecular Systems examines systematic ways of constructing coarse grained representations for complex systems It explains how this approach can be used in the simulation and modeling of condensed phase and biomolecular systems Assembling some of the most influential world renowned researchers in the field this book covers the latest developments in the coarse grained molecular dynamics simulation and modeling of condensed phase and biomolecular systems Each chapter focuses on specific examples of evolving coarse graining methodologies and presents results for a variety of complex systems The contributors discuss the minimalist inversion and multiscale approaches to coarse graining along with the emerging challenges of coarse graining They also connect atomic level information with new coarse grained representations of complex systems such as lipid bilayers proteins peptides and DNA

Computational Approaches in Physics Maria Fyta, 2016-11-01 Computational Approaches in Physics reviews computational schemes which are used in the simulations of physical systems These range from very accurate ab initio techniques up to coarse grained and mesoscopic schemes The choice of the method is based on the desired accuracy and computational efficiency A bottom up approach is used to present the various simulation methods used in Physics starting from the lower level and the most accurate methods up to particle based ones The book outlines the basic theory underlying each technique and its complexity addresses the computational implications and issues in the implementation as well as present representative examples A link to the most common computational codes commercial or open source is listed in each chapter The strengths and deficiencies of the variety of techniques discussed in this book are presented in detail and visualization tools commonly used to make the simulation data more comprehensive are also discussed In the end specific techniques are used as bridges across different disciplines To this end examples of different systems tackled with the same methods are presented The appendices include elements of physical theory which are prerequisites in understanding the simulation methods

Coarse-Grained Modeling of Biomolecules Gargi A. Papoian, 2017-10-30 The chapters in this book survey the progress in simulating biomolecular dynamics The images conjured up by this work are not yet universally loved but are beginning to bring new insights into the study of biological structure and function The future will decide whether this scientific movement can bring forth its Picasso or Modigliani from the Foreword by Peter G Wolynes Bullard Welch Foundation Professor of Science Rice University This book highlights the state of art in coarse grained modeling of biomolecules covering both fundamentals as well as various cutting edge applications Coarse graining of biomolecules is an area of rapid advances with numerous new force fields having appeared recently and significant progress made in developing a systematic theory of coarse graining The contents start with first fundamental principles based on physics then survey specific state of art coarse grained force fields of proteins and nucleic acids and provide examples of exciting biological

problems that are at large scale and hence only amenable to coarse grained modeling Introduces coarse grained models of proteins and nucleic acids Showcases applications such as genome packaging in nuclei and understanding ribosome dynamics Gives the physical foundations of coarse graining Demonstrates use of models for large scale assemblies in modern studies Garegin A Papoian is the first Monroe Martin Associate Professor with appointments in the Department of Chemistry and Biochemistry and the Institute for Physical Science and Technology at the University of Maryland

Hierarchical Methods for Dynamics in Complex Molecular Systems Johannes Grotendorst, 2012 Advances in Physical Organic Chemistry, 2020-10-22 Advances in Physical Organic Chemistry Volume 54 presents the latest reviews of recent work in physical organic chemistry The book provides a valuable source of information that is ideal not only for physical organic chemists applying their expertise to both novel and traditional problems but also for non specialists across diverse areas who identify a physical organic component in their approach to research Its hallmark is a quantitative molecular level understanding of phenomena across a diverse range of disciplines Reviews the application of quantitative and mathematical methods to help readers understand chemical problems Provides the chemical community with authoritative and critical assessments of the many aspects of physical organic chemistry Covers organic organometallic bioorganic enzymes and materials topics Presents the only regularly published resource for reviews in physical organic chemistry Written by authoritative experts who cover a wide range of topics that require a quantitative molecular level understanding of phenomena across a diverse range of disciplines

Computational Approaches for Understanding Dynamical Systems: Protein Folding and Assembly, 2020-03-05 Computational Approaches for Understanding Dynamical Systems Protein Folding and Assembly Volume 170 in the Progress in Molecular Biology and Translational Science series provides the most topical informative and exciting monographs available on a wide variety of research topics The series includes in depth knowledge on the molecular biological aspects of organismal physiology with this release including chapters on Pairwise Additive and Polarizable Atomistic Force Fields for Molecular Dynamics Simulations of Proteins Scale consistent approach to the derivation of coarse grained force fields for simulating structure dynamics and thermodynamics of biopolymers Enhanced sampling and free energy methods and much more Includes comprehensive coverage on molecular biology Presents ample use of tables diagrams schemata and color figures to enhance the reader's ability to rapidly grasp the information provided Contains contributions from renowned experts in the field

Computational Pharmaceutics Defang Ouyang, Sean C. Smith, 2015-07-20 Molecular modeling techniques have been widely used in drug discovery fields for rational drug design and compound screening Now these techniques are used to model or mimic the behavior of molecules and help us study formulation at the molecular level Computational pharmaceutics enables us to understand the mechanism of drug delivery and to develop new drug delivery systems The book discusses the modeling of different drug delivery systems including cyclodextrins solid dispersions polymorphism prediction dendrimer based delivery systems surfactant based micelle

polymeric drug delivery systems liposome protein peptide formulations non viral gene delivery systems drug protein binding silica nanoparticles carbon nanotube based drug delivery systems diamond nanoparticles and layered double hydroxides LDHs drug delivery systems Although there are a number of existing books about rational drug design with molecular modeling techniques these techniques still look mysterious and daunting for pharmaceutical scientists This book fills the gap between pharmaceutics and molecular modeling and presents a systematic and overall introduction to computational pharmaceutics It covers all introductory advanced and specialist levels It provides a totally different perspective to pharmaceutical scientists and will greatly facilitate the development of pharmaceutics It also helps computational chemists to look for the important questions in the drug delivery field This book is included in the Advances in Pharmaceutical Technology book series Self-Assembly of Nanostructures and Patchy Nanoparticles Shafigh Mehraeen,2020-11-04 Top down approaches are currently the main contributor of fabricating microelectronic devices However the prohibitive cost of numerous technological steps in these approaches is the main obstacle to further progress Furthermore a large number of applications necessitate fabrication of complex and ultra small devices that cannot be made using these approaches New approaches based on natural self assembly of matter need to be developed to allow for fabrication of micro and nanoelectronic devices Self assembly of nanostructures is a dynamic field which explores physics of these structures and new ways to fabricate them However the major problem is how to control the properties of the nanostructures resulting from low dimensionality This book presents recent advances made to address this problem and fabricate nanostructures using self assembly **Computational Chemistry Methods in Structural Biology** Christo Christov,2011-09-23 Published continuously since 1944 the Advances in Protein Chemistry and Structural Biology serial has been a continuous essential resource for protein chemists Covering reviews of methodology and research in all aspects of protein chemistry including purification expression proteomics modeling and structural determination and design each volume brings forth new information about protocols and analysis of proteins while presenting the most recent findings from leading experts in a broad range of protein related topics This volume features articles on Computational Chemistry methods in Structural Biology Essential resource for protein chemists This volume features articles on Computational Chemistry methods in Structural Biology *Advancing Theory for Kinetics and Dynamics of Complex, Many-Dimensional Systems* Tamiki Komatsuzaki,R. Stephen Berry,David M. Leitner,2011-07-07 This series provides the chemical physics field with a forum for critical authoritative evaluations of advances in every area of the discipline Volume 145 in the series continues to report recent advances with significant up to date chapters by internationally recognized researchers

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