



George Khelashvili

Theoretical and Simulation Study of Lipid Membranes

Application to Lipid Rafts

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Joacim Rocklöv



Theoretical And Simulation Study Of Lipid Membranes Application To Lipid Rafts:

Biophysical Approaches for the Study of Membrane Structure Part B, 2024-07-21 *Biophysical Approaches for the Study of Membrane Structure Part B* Volume 701 explores lipid membrane asymmetry and lateral heterogeneity A burst of recent research has shown that bilayers whose leaflets differ in their physical properties such as composition phase state or lateral stress exhibit many fascinating new characteristics but also pose a host of challenges related to their creation characterization simulation and theoretical description Chapters in this new release include Characterization of domain formation in complex membranes Analyzing the bending modulus from simulations of complex membranes The density threshold affinity Calculating lipid binding affinities from unbiased Coarse Grain Molecular Dynamics simulations and much more Additional sections cover Uncertainty quantification for trans membrane stresses and moments from simulation Using molecular dynamics simulations to generate small angle scattering curves and cryo EM images of proteoliposomes Binary Bilayer Simulations for Partitioning Within Membranes Modeling Asymmetric Cell Membranes at All atom Resolution Multiscale remodeling of biomembranes and vesicles Building complex membranes with Martini 3 Predicting lipid sorting in curved bilayer membranes Simulating asymmetric membranes using P21 periodic boundary conditions and many other interesting topics Explore the state of the art of lipid membrane asymmetry Covers experimental theoretical and computational techniques to create and characterize asymmetric lipid membranes Teaches how these kinds of approaches create and characterize laterally inhomogeneous membranes

Combining Simulations, Theory, and Experiments into Multiscale Models of Biological Events Fabio Trovato, Peter J. Bond, Joanna Trylska, Peter Guy Wolynes, 2022-01-11

Applications of Density Functional Theory to Biological and Bioinorganic Chemistry Mihai V. Putz, D Michael P Mingos, 2013-02-01 The series *Structure and Bonding* publishes critical reviews on topics of research concerned with chemical structure and bonding The scope of the series spans the entire Periodic Table and addresses structure and bonding issues associated with all of the elements It also focuses attention on new and developing areas of modern structural and theoretical chemistry such as nanostructures molecular electronics designed molecular solids surfaces metal clusters and supramolecular structures Physical and spectroscopic techniques used to determine examine and model structures fall within the purview of *Structure and Bonding* to the extent that the focus is on the scientific results obtained and not on specialist information concerning the techniques themselves Issues associated with the development of bonding models and generalizations that illuminate the reactivity pathways and rates of chemical processes are also relevant The individual volumes in the series are thematic The goal of each volume is to give the reader whether at a university or in industry a comprehensive overview of an area where new insights are emerging that are of interest to a larger scientific audience Thus each review within the volume critically surveys one aspect of that topic and places it within the context of the volume as a whole The most significant developments of the last 5 to 10 years should be presented using selected examples to illustrate

the principles discussed A description of the physical basis of the experimental techniques that have been used to provide the primary data may also be appropriate if it has not been covered in detail elsewhere The coverage need not be exhaustive in data but should rather be conceptual concentrating on the new principles being developed that will allow the reader who is not a specialist in the area covered to understand the data presented Discussion of possible future research directions in the area is welcomed Review articles for the individual volumes are invited by the volume editors Readership research scientists at universities or in industry graduate students Special offer For all customers who have a standing order to the print version of Structure and Bonding we offer free access to the electronic volumes of the Series published in the current year via SpringerLink

From Single Molecules to Nanoscopically Structured Materials Thomas Basché, Klaus Müllen, Manfred Schmidt, 2014-06-03 Mechanical Properties of Single Molecules and Polymer Aggregates R diger Berger Kurt Binder Gregor Diezemann J rgen Gau Mark Helm Katharina Landfester Wolfgang Paul Halle Peter Virnau Optical Properties of Individual Molecular Aggregates and Nano Particles Thomas Basch Hans J rgen Butt Gregor Diezemann J rgen Gau Klaus M llen Harald Paulsen Carsten S nnichsen Rudolf Zentel Structure Formation of Polymeric Building Blocks I Self assembly of Copolymers Kurt Binder Holger Frey Andreas Kilbinger Univ Fribourg Ute Kolb Michael Maskos IMM Mainz Wolfgang Paul Univ Halle Hans Wolfgang Spiess Structure Formation of Polymeric Building Blocks II Complex Polymer Architectures Kurt Binder Hans J rgen Butt Angelika K hnle Klaus M llen Wolfgang Paul Univ Halle Erwin Schmidt Manfred Schmidt Hans Wolfgang Spiess Thomas Vilgis Structure Formation of Polymeric Building Blocks III Polymer Complexes in Biological Applications Kurt Kremer Heiko Luhmann Christine Peter Friederike Schmid Erwin Schmidt Manfred Schmidt Eva Sinner Univ of Natural Resources Vienna Tanja Weil Univ Ulm

A Systems Biology Approach to Study Metabolic Syndrome Matej Orešič, Antonio Vidal-Puig, 2013-09-24 The aim of this book is to provide the target audience specifically students of Medicine Biology Systems Biology and Bioinformatics as well as experienced researchers in research fields relevant to metabolic syndrome MetS with an overview of the challenges and opportunities in systems biology and how it can be used to tackle MetS In particular the aims are 1 to provide an introduction to the key biological processes involved in the pathophysiology of MetS 2 through the use of specific examples provide an introduction to the latest technologies that use a systems biology approach to study MetS and 3 to give an overview of the mathematical modeling approaches for studying MetS The clearly written chapters by leading experts in the field provides detailed descriptions crucial for the unique position of this book and its focus on the application of systems biology to tackle specific pathophysiologically relevant aspects of MetS and provides a valuable practical guide to this research community

Computational Methods to Study the Structure and Dynamics of Biomolecules and Biomolecular Processes Adam Liwo, 2018-12-19 This book provides a comprehensive overview of modern computer based techniques for analyzing the structure properties and dynamics of biomolecules and biomolecular processes It is organized in four main parts the first one deals with methodology of molecular simulations the second one with

applications of molecular simulations the third one introduces bioinformatics methods and the use of experimental information in molecular simulations the last part reports on selected applications of molecular quantum mechanics This second edition has been thoroughly revised and updated to include the latest progresses made in the respective field of research Computational Pharmaceutics Defang Ouyang, Sean C. Smith, 2015-05-19 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 Advances in Planar Lipid Bilayers and Liposomes Ales Iglic, 2011-10-04 Advances in Planar Lipid Bilayers and Liposomes volumes cover a broad range of topics including main arrangements of the reconstituted system namely planar lipid bilayers as well as spherical liposomes The invited authors present the latest results of their own research groups in this exciting multidisciplinary field Incorporates contributions from newcomers and established and experienced researchers Explores the planar lipid bilayer systems and spherical liposomes from both theoretical and experimental perspectives Serves as an indispensable source of information for new scientists

Comprehensive Biophysics, 2012-04-12 Biophysics is a rapidly evolving interdisciplinary science that applies theories and methods of the physical sciences to questions of biology Biophysics encompasses many disciplines including physics chemistry mathematics biology biochemistry medicine pharmacology physiology and neuroscience and it is essential that scientists working in these varied fields are able to understand each other's research Comprehensive Biophysics Nine Volume Set will help bridge that communication gap Written by a team of researchers at the forefront of their respective fields under the guidance of Chief Editor Edward Egelman Comprehensive Biophysics Nine Volume Set provides definitive introductions to a broad array of topics uniting different areas of biophysics research from the physical techniques for studying macromolecular structure to protein folding muscle and molecular motors cell biophysics bioenergetics and more

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Modeling Biomaterials Josef Málek, Endre Süli, 2022-01-21. The investigation of the role of mechanical and mechano chemical interactions in cellular processes and tissue development is a rapidly growing research field in the life sciences and in biomedical engineering. Quantitative understanding of this important area in the study of biological systems requires the development of adequate mathematical models for the simulation of the evolution of these systems in space and time. Since expertise in various fields is necessary this calls for a multidisciplinary approach. This edited volume connects basic physical biological and physiological concepts to methods for the mathematical modeling of various materials by pursuing a multiscale approach from subcellular to organ and system level. Written by active researchers each chapter provides a detailed introduction to a given field illustrates various approaches to creating models and explores recent advances and future research perspectives. Topics covered include molecular dynamics simulations of lipid membranes phenomenological continuum mechanics of tissue growth and translational cardiovascular modeling. Modeling Biomaterials will be a valuable resource for both non specialists and experienced researchers from various domains of science such as applied mathematics biophysics computational physiology and medicine.

Frontiers in Computational Chemistry: Volume 2 Zaheer Ul-Haq, Jeffry D. Madura, 2015-12-16. Frontiers in Computational Chemistry originally published by Bentham and now distributed by Elsevier presents the latest research findings and methods in the diverse field of computational chemistry focusing on molecular modeling techniques used in drug discovery and the drug development process. This includes computer aided molecular design drug discovery and development lead generation lead optimization database management computer and molecular graphics and the development of new computational methods or efficient algorithms for the simulation of chemical phenomena including analyses of biological activity. In Volume 2 the authors continue the compendium with nine additional perspectives in the application of

computational methods towards drug design This volume covers an array of subjects from modern hardware advances that accelerate new antibacterial peptide identification electronic structure methods that explain how singlet oxygen damages DNA to QSAR model validation the application of DFT and DFRT methods on understanding the action of nitrogen mustards the design of novel prodrugs using molecular mechanics and molecular orbital methods computational simulations of lipid bilayers high throughput screening methods and more Brings together a wide range of research into a single collection to help researchers keep up with new methods Uniquely focuses on computational chemistry approaches that can accelerate drug design Makes a solid connection between experiment and computation and the novel application of computational methods in the fields of biology chemistry biochemistry physics and biophysics

Polymer Science: A Comprehensive Reference ,2012-12-05 The progress in polymer science is revealed in the chapters of Polymer Science A Comprehensive Reference Ten Volume Set In Volume 1 this is reflected in the improved understanding of the properties of polymers in solution in bulk and in confined situations such as in thin films Volume 2 addresses new characterization techniques such as high resolution optical microscopy scanning probe microscopy and other procedures for surface and interface characterization Volume 3 presents the great progress achieved in precise synthetic polymerization techniques for vinyl monomers to control macromolecular architecture the development of metallocene and post metallocene catalysis for olefin polymerization new ionic polymerization procedures and atom transfer radical polymerization nitroxide mediated polymerization and reversible addition fragmentation chain transfer systems as the most often used controlled living radical polymerization methods Volume 4 is devoted to kinetics mechanisms and applications of ring opening polymerization of heterocyclic monomers and cycloolefins ROMP as well as to various less common polymerization techniques Polycondensation and non chain polymerizations including dendrimer synthesis and various click procedures are covered in Volume 5 Volume 6 focuses on several aspects of controlled macromolecular architectures and soft nano objects including hybrids and bioconjugates Many of the achievements would have not been possible without new characterization techniques like AFM that allowed direct imaging of single molecules and nano objects with a precision available only recently An entirely new aspect in polymer science is based on the combination of bottom up methods such as polymer synthesis and molecularly programmed self assembly with top down structuring such as lithography and surface templating as presented in Volume 7 It encompasses polymer and nanoparticle assembly in bulk and under confined conditions or influenced by an external field including thin films inorganic organic hybrids or nanofibers Volume 8 expands these concepts focusing on applications in advanced technologies e g in electronic industry and centers on combination with top down approach and functional properties like conductivity Another type of functionality that is of rapidly increasing importance in polymer science is introduced in volume 9 It deals with various aspects of polymers in biology and medicine including the response of living cells and tissue to the contact with biofunctional particles and surfaces The last volume is devoted to the scope and potential

provided by environmentally benign and green polymers as well as energy related polymers They discuss new technologies needed for a sustainable economy in our world of limited resources Provides broad and in depth coverage of all aspects of polymer science from synthesis polymerization properties and characterization methods and techniques to nanostructures sustainability and energy and biomedical uses of polymers Provides a definitive source for those entering or researching in this area by integrating the multidisciplinary aspects of the science into one unique up to date reference work Electronic version has complete cross referencing and multi media components Volume editors are world experts in their field including a Nobel Prize winner

International Perspectives on Science Education for the Gifted Keith Taber, Manabu Sumida, 2016-04-28 In the spirit of encouraging international dialogue between researchers and practitioners often working within isolated traditions this book discusses perspectives on science education for the gifted informed by up to date research findings from a number of related fields The book reviews philosophy culture and programmes in science education for the gifted in diverse national contexts and includes scholarly reviews of significant perspectives and up to date research methods and findings The book is written in a straightforward style for students studying international perspective modules on undergraduate but especially masters and doctoral degrees in Science Education and Gifted Education Gifted education has come to be regarded as a key national programme in many countries and gifted education in science disciplines is now of major importance to economic and technological development Despite these national initiatives and developments there are very few discussions on gifted education in science from international perspectives This will be a valued addition to the scholarship in this emergent field

Liposomes, Lipid Bilayers and Model Membranes Georg Pabst, Norbert Kučerka, Mu-Ping Nieh, John Katsaras, 2014-03-04 As a result of their unique physical properties biological membrane mimetics such as liposomes are used in a broad range of scientific and technological applications Liposomes Lipid Bilayers and Model Membranes From Basic Research to Application describes state of the art research and future directions in the field of membranes which has evolved from basic studies of the physicochemical properties of amphiphiles to their application in industry and medicine Written by leading researchers in their fields this book describes basic and applied research and serves as a useful reference for both the novice and the expert Part one covers a range of basic research topics from theory and computational simulations to some of the most up to date experimental research Topics discussed include soft matter physics of membranes nonlamellar phases extraction of molecules by amphiphiles lipid models for membrane rafts membrane dynamics nanodiscs microemulsions active membranes as well as interactions of bilayers with drugs or DNA to treat disease or for gene transfer respectively Part two of the book focuses on technological applications of amphiphiles such as liposome based nanoparticles for drug delivery formulation of liposomes for prolonged in vivo circulation and functionalization for medical purposes novel drug delivery systems for increased drug loading and the use of tethered membranes for bio sensing applications Chapters also describe the use of liposomes in textile dyeing and how lipidic

nanoparticles are used by the food industry **Molecular Dynamics and Machine Learning in Drug Discovery** Sergio Decherchi, Andrea Cavalli, Pratyush Tiwary, Francesca Grisoni, 2021-06-08 Dr Sergio Decherchi and Dr Andrea Cavalli are co founders of BiKi Technologies s r l a company that commercializes a Molecular Dynamics based software suite for drug discovery All other Topic Editors declare no competing interests with regards to the Research Topic subject

Characterization of Biological Membranes Mu-Ping Nieh, Frederick A. Heberle, John Katsaras, 2019-07-22 The study of membranes has become of high importance in the fields of biology pharmaceutical chemistry and medicine since much of what happens in a cell or in a virus involves biological membranes The current book is an excellent introduction to the area which explains how modern analytical methods can be applied to study biological membranes and membrane proteins and the bioprocesses they are involved to Functional Heterogeneities in Biomembranes Rainer A. Böckmann, Robert

Ernst, Falk Nimmerjahn, 2021-09-01 **Annual Reports in Computational Chemistry** Ralph A. Wheeler, 2014-12-03 Annual Reports in Computational Chemistry provides timely and critical reviews of important topics in computational chemistry as applied to all chemical disciplines Topics covered include quantum chemistry molecular mechanics force fields chemical education and applications in academic and industrial settings Focusing on the most recent literature and advances in the field each article covers a specific topic of importance to computational chemists Quantum chemistry Molecular mechanics Force fields Chemical education and applications in academic and industrial settings **Advances in Planar Lipid Bilayers and Liposomes** Aleš Iglič, 2012-08-06 Advances in Planar Lipid Bilayers and Liposomes volumes cover a broad range of topics including main arrangements of the reconstituted system namely planar lipid bilayers as well as spherical liposomes The invited authors present the latest results of their own research groups in this exciting multidisciplinary field Incorporates contributions from newcomers and established and experienced researchers Explores the planar lipid bilayer systems and spherical liposomes from both theoretical and experimental perspectives Serves as an indispensable source of information for new scientists *NIC Symposium 2010* John-von-Neumann-Institut für Computing (Jülich), 2010

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