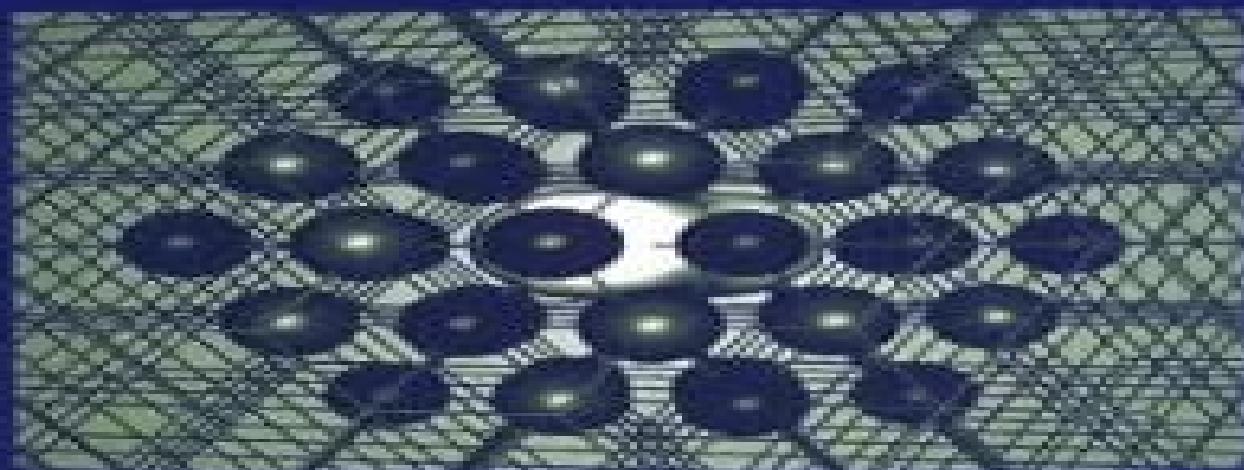


Molecular Modeling Applications in Crystallization



Edited by Allan S. Myerson

Molecular Modeling Applications In Crystallization

Lena Ohannesian,Anthony Streeter



Molecular Modeling Applications In Crystallization:

Molecular Modeling Applications in Crystallization Allan S. Myerson, 1999-06-28 Crystallization is an important purification process used in a broad range of industries including pharmaceuticals foods and bulk chemicals In recent years molecular modeling has emerged as a useful tool in the analysis and solution of problems associated with crystallization Modeling allows more focused experimentation based on structural and energetic calculations instead of intuition and trial and error This book offers a general introduction to molecular modeling techniques and their application in crystallization After explaining the basic concepts of molecular modeling and crystallization the book discusses how modeling techniques are used to solve a variety of practical problems related to crystal size shape internal structure and properties With chapters written by leading experts and an emphasis on problem solving this book will appeal to scientists engineers and graduate students involved in research and the production of crystalline materials

Molecular Modeling for the Design of Novel Performance Chemicals and Materials Beena Rai, 2012-03-23 Molecular modeling MM tools offer significant benefits in the design of industrial chemical plants and material processing operations While the role of MM in biological fields is well established in most cases MM works as an accessory in novel products materials development rather than a tool for direct innovation As a result MM engineers and

Crystallization and Solidification Properties of Lipids Neil Widlak, Richard W. Hartel, Suresh Narine, 2001 Annotation The crystallization and solidification properties of lipids influence their functional properties in biological systems foods personal care products pharmaceuticals and oleo chemicals To help its members and others optimize products or systems containing lipids the American Oil Chemists Society devoted its 2000 conference held in Toronto to the fundamental principles of lipid crystallization The resulting 20 papers discuss phase behavior and polymorphism lipid crystallization kinetics microstructure and rheology and crystallization in emulsions They also consider applications to dairy systems manufacturing chocolate confection and the texture of fats Annotation c Book News Inc Portland OR booknews com

Handbook of Industrial Crystallization Allan Myerson, 2002-01-08 Crystallization is an important separation and purification process used in industries ranging from bulk commodity chemicals to specialty chemicals and pharmaceuticals In recent years a number of environmental applications have also come to rely on crystallization in waste treatment and recycling processes The authors provide an introduction to the field of newcomers and a reference to those involved in the various aspects of industrial crystallization It is a complete volume covering all aspects of industrial crystallization including material related to both fundamentals and applications This new edition presents detailed material on crystallization of biomolecules precipitation impurity crystal interactions solubility and design Provides an ideal introduction for industrial crystallization newcomers Serves as a worthwhile reference to anyone involved in the field Covers all aspects of industrial crystallization in a single complete volume

Purification of Biotechnological Products Adalberto Pessoa Jr, Beatriz Vahan Kilikian, Paul Long, 2024-05-23 This outstanding text focuses on providing professionals

and students working in the pharmaceutical and biotechnology field with the background necessary for developing of a product or process and with the necessary rigor required by federal regulatory agencies in the pharmaceutical industry The material will enable teachers lecturers and professors in biotechnology to prepare courses on basic concepts and applications for the purification of biotechnological products of industrial interest These can be applied in practice for example with projects on purification development on an industrial scale or useful unit operations for the development of bioproducts of commercial interest Features Purification and development of new bioproducts and improvement of those being produced Provides a background and concepts on the purification of biomolecules and with an industrial perspective It allows professionals to understand the entire process of developing a biopharmaceutical or bio food from bench to industry in biotechnology one of the fastest growing sectors of the economy It promotes the dissemination of information in a didactic way which is of paramount importance for interdisciplinary fields It enables the reader to follow step by step stages of the development of a new biopharmaceutical and allows the optimization of existing processes

Reviews in Computational Chemistry, Volume 17 Kenny B. Lipkowitz, Donald B. Boyd, 2003-04-24 Computational chemistry is increasingly used in most areas of molecular science including organic inorganic medicinal biological physical and analytical chemistry Researchers in these fields who do molecular modelling need to understand and stay current with recent developments This volume like those prior to it features chapters by experts in various fields of computational chemistry Two chapters focus on molecular docking one of which relates to drug discovery and cheminformatics and the other to proteomics In addition this volume contains tutorials on spin orbit coupling and cellular automata modeling as well as an extensive bibliography of computational chemistry books FROM REVIEWS OF THE SERIES Reviews in Computational Chemistry remains the most valuable reference to methods and techniques in computational chemistry JOURNAL OF MOLECULAR GRAPHICS AND MODELLING One cannot generally do better than to try to find an appropriate article in the highly successful Reviews in Computational Chemistry The basic philosophy of the editors seems to be to help the authors produce chapters that are complete accurate clear and accessible to experimentalists in particular and other nonspecialists in general JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

Materials Science and Applied Chemistry IV M̄aris Turks, 2021-11-10 Selected peer reviewed full text papers from the 61st conference Materials Science and Applied Chemistry MSAC 2020 Selected peer reviewed papers from the 61st conference Materials Science and Applied Chemistry MSAC 2020 23 October 2020 Riga Latvia

Modern Aspects of Bulk Crystal and Thin Film Preparation Nikolai Kolesnikov, Elena Borisenko, 2012-01-13 In modern research and development materials manufacturing crystal growth is known as a way to solve a wide range of technological tasks in the fabrication of materials with preset properties This book allows a reader to gain insight into selected aspects of the field including growth of bulk inorganic crystals preparation of thin films low dimensional structures crystallization of proteins and other organic compounds

Design and Processing of Particulate Products Jim

Litster,2016-10-20 With this unique and comprehensive text readers will gain the quantitative tools needed to engineer the particulate processes and products that are ubiquitous in modern life Covering a series of particle and particulate delivery form design processes with emphasis on design and operation to control particle attributes and supported by many worked examples it is essential reading for students and practitioners Topics covered include a range of particle design processes such as crystallization and precipitation granulation grinding aerosol processes and spray drying as well as forms of delivery such as granules tablets dry powders and aerosols Readers will learn from real world examples how the primary particle properties and the structure and properties of the delivery form can lead to high performance products ranging from pharmaceuticals consumer goods and foods to specialty chemicals paints agricultural chemicals and minerals

Cheminformatics Developments Jan H. Noordik,2004 The developments in information technology in the last decades of the 20th century have fundamentally changed the way in which scientific information is being communicated and used A scientific discipline where the impact of these changes has been particularly significant is bio chemistry Up to less than 25 years ago molecular modeling was a hardly existent computational chemistry niche only practiced at those few institutes that could afford the very expensive specialised hardware Also rapid access to not only the primary literature but possibly even more importantly to the factual primary data about millions of chemical compounds to reactions structures and spectra and to the genomic data of various organisms including humans can only be provided by digital storage and retrieval techniques This book seeks to document some key developments in computerized chemical information in the last two decades of the past century To put the developments into a historic perspective the three opening chapters present review articles on the founding the history and the operation of three different representative European computer chemistry institutes These introductory chapters are personal accounts of history and development and clearly show the different approaches and aims in setting up these academic research and or service facilities for computer aided chemistry and cheminformatics The following chapters form a bridge to recent cheminformatics research by covering selected topics in the fields of organic synthesis drug design crystallography modeling and chemistry teaching European Symposium on Computer Aided

Process Engineering - 14 Ana Paula Barbosa-Póvoa,Henrique Matos,2004-05-14 This book contains papers presented at the 14th European Symposium on Computer Aided Process Engineering ESCAPE 14 The ESCAPE symposia bring together scientists students and engineers from academia and industry who are active in the research and application of Computer Aided Process Engineering The objective of ESCAPE 14 is to highlight the use of computers and information technology tools on five specific themes 1 Product and Process Design 2 Synthesis and Process Integration 3 Process Control and Analysis 4 Manufacturing Process Operations 5 New Challenges in CAPE Provides this year s comprehensive overview of the current state of affairs in the CAPE community Contains reports from the frontiers of science by the field s most respected scientists Special Keynote by Professor Roger Sargent Long Term Achievement CAPE Award winner **Energetic Materials** Ulrich

Teipel,2006-03-06 Incorporation of particular components with specialized properties allows one to tailor the end product s properties For instance the sensitivity burning behavior thermal or mechanical properties or stability of energetic materials can be affected and even controllably varied through incorporation of such ingredients This book examines particle technologies as applied to energetic materials such as propellants and explosives thus filling a void in the literature on this subject Following an introduction covering general features of energetic materials the first section of this book describes methods of manufacturing particulate energetic materials including size reduction crystallization atomization particle formation using supercritical fluids and microencapsulation agglomeration phenomena special considerations in mixing explosive particles and the production of nanoparticles The second section discusses the characterization of particulate materials Techniques and methods such as particle size analysis morphology elucidation and the determination of chemical and thermal properties are presented The wettability of powders and rheological behavior of suspensions and solids are also considered Furthermore methods of determining the performance of particular energetic materials are described Each chapter deals with fundamentals and application possibilities of the various methods presented with particular emphasis on issues applicable to particulate energetic materials The book is thus equally relevant for chemists physicists material scientists chemical and mechanical engineers and anyone interested or engaged in particle processing and characterization technologies

The Chemistry of Nanostructured Materials Peidong Yang,2003 This book is a sequel to the first volume of The Chemistry of Nanostructured Materials It covers the most exciting developments in the nanostructured materials field for the past five to ten years with a particular focus on their applications in energy conversion and energy storage Prominent authors of recognized authority in the field contribute their expertise in the review chapters Book Jacket *Bioinspiration*

Xiang Yang Liu,2012-12-09 Methods in bioinspiration and biomimicking have been around for a long time However due to current advances in modern physical biological sciences and technologies our understanding of the methods have evolved to a new level This is due not only to the identification of mysterious and fascinating phenomena but also to the understandings of the correlation between the structural factors and the performance based on the latest theoretical modeling and experimental technologies Bioinspiration From Nano to Micro Scale provides readers with a broad view of the frontiers of research in the area of bioinspiration from the nano to macroscopic scales particularly in the areas of biomineralization antifreeze protein and antifreeze effect It also covers such methods as the lotus effect and superhydrophobicity structural colors in animal kingdom and beyond as well as behavior in ion channels A number of international experts in related fields have contributed to this book which offers a comprehensive and synergistic look into challenging issues such as theoretical modeling advanced surface probing and fabrication The book also provides a link to the engineering of novel advanced materials playing an important role in advancing technologies in various fields

Synchrotron Radiation and Structural Proteomics Eugenia Pechkova,Christian Riek,2011-11-11 This book presents an overview of the current state of research in

both synchrotron radiation and structural proteomics from different laboratories worldwide The book presents recent research results in the most advanced methods of synchrotron radiation analysis protein micro and nano crystallography X ray scattering and X ray optics coherent

The Philosophy of Chemistry Jean-Pierre Llored, 2014-09-26 This volume connects chemistry and philosophy in order to face questions raised by chemistry in our present world The idea is first to develop a kind of philosophy of chemistry which is deeply rooted in the exploration of chemical activities We thus work in close contact with chemists technicians engineers researchers and teachers Following this line of reasoning the first part of the book encourages current chemists to describe their workaday practices while insisting on the importance of attending to methodological metrological philosophical and epistemological questions related to their activities It deals with sustainable chemistry chemical metrology nanochemistry and biochemistry among other crucial topics In doing so those chemists invite historians and philosophers to provide ideas for future developments In a nutshell this part is a call for forthcoming collaborations focused on instruments and methods that is on ways of doing chemistry The second part of the book illustrates the multifarious ways to study chemistry and even proposes new approaches to doing so Each approach is interesting and incomplete but the emergent whole is richer than any of its components Analytical work needs socio historical expertise as well as many other approaches in order to keep on investigating chemistry to greater and greater depth This heterogeneity provides a wide set of methodological perspectives not only about current chemical practices but also about the ways to explore them philosophically Each approach is a resource to study chemistry and to reflect upon what doing philosophy of science can mean In the last part of the volume philosophers and chemists propose new concepts or reshape older ones in order to think about chemistry The act of conceptualization itself is queried as well as the relationships between concepts and chemical activities Prefaced by Nobel Laureate in Chemistry Roald Hoffmann and by the President of the International Society for the Philosophy of Chemistry Rom Harr this volume is a plea for the emergence of a collective cleverness and aims to foster inventiveness

Crystal Growth of Organic Materials Allan S. Myerson, Daniel A. Green, Paul Meenan, 1996 Examines emerging technologies in the use of crystallization as a purification and separation process in the food pharmaceutical and commodity and specialty chemical industries Discusses the application of molecular modelling and calculation chemistry to crystallization Includes chapters focusing on crystal morphology and chirality

Foundations of Molecular Modeling and Simulation Randall Q Snurr, Claire S. Adjiman, David A. Kofke, 2016-06-01 This book is a collection of select proceedings of the FOMMS 2015 conference FOMMS 2015 was the sixth triennial FOMMS conference showcasing applications of theory of computational quantum chemistry molecular science and engineering simulation The theme of the 2015 meeting was on Molecular Modeling and the Materials Genome This volume comprises chapters on many distinct applications of molecular modeling techniques The content will be useful to researchers and students alike

Macroeconomics for Business and Society Francis Gerard Adams, 2002 In recent years the world economy has been

undergoing drastic changes the East Asian miracle the financial crisis and today globalization and the fundamental changes associated with the new economy This book integrates these developments with macroeconomics for business managers and policymakers Macroeconomics is essential background for the business manager and policymaker Consequently macroeconomics is an integral part of the business curriculum in mature and developing countries alike And well it should be The economy affects decisions by investors manufacturers distributors importers and exporters etc in all parts of the world Often it is the difference between growth and profitability on one hand and stagnation or failure on the other In recent years as the world economy has undergone overwhelming changes especially in East Asia and now in the advanced countries understanding what is going on in the local economy and out there in the world has become a particular challenge to managers The new developments of which the new economy is the most recent one do not supercede the basic theoretical framework of macroeconomics But they add greatly to the challenge of understanding the economic situation and to its uncertainty This book was originally written to meet the needs of a business curriculum based on the program at the Sasin Graduate Institute of Business Administration of Chulalongkorn University in Bangkok in collaboration with the Wharton and Kellogg Business Schools in the United States The book is intended for a broad audience both domestic and international that includes mature MBA business students intermediate level undergraduates and informed laypersons Handbook of Pharmaceutical Analysis Lena Ohannesian,Anthony Streeter,2001-11-09 Exploring the analysis of pharmaceuticals including polymorphic forms this book discusses regulatory requirements in pharmaceutical product development and pharmaceutical testing It covers methods of drug separation and procedures such as capillary electrophoresis for chromatographic separation of molecules Additional topics include drug formulation analysis using vibrational and magnetic resonance spectroscopy and identification of drug metabolites and decomposition products using such techniques as mass spectrometry The book provides more than 300 tables equations drawings and photographs and convenient easy to use indices facilitating quick access to each topic

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