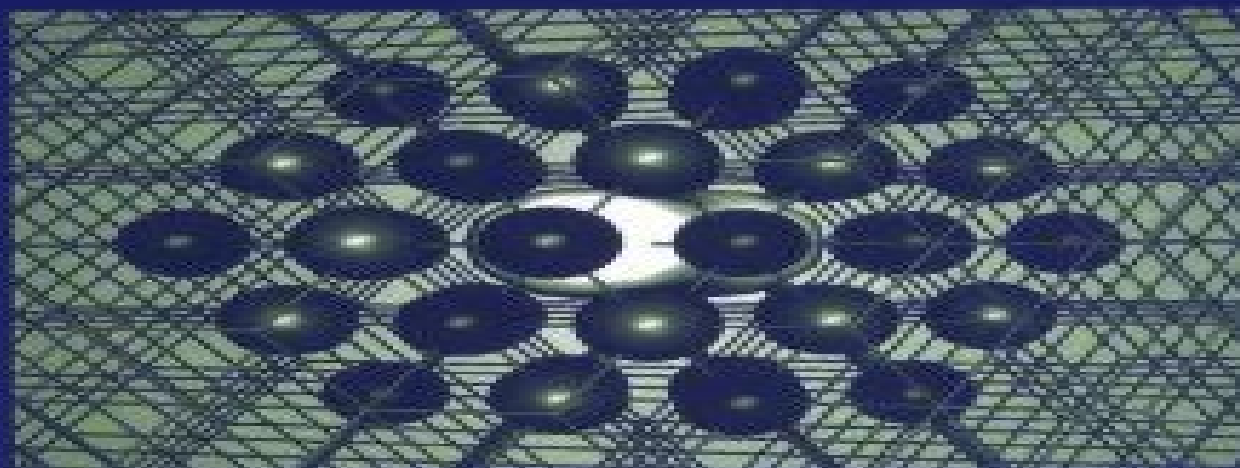


Molecular Modeling Applications in Crystallization



Edited by Allan S. Myerson

Molecular Modeling Applications In Crystallization

Jan H. Noordik



Molecular Modeling Applications In Crystallization:

Molecular Modeling Applications in Crystallization Allan S. Myerson,1999-06-28 The first book to introduce molecular modeling and its applications in crystallization written by leading experts in the field **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 **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 Māris 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 *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

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

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

Cellulose Chemistry and Technology, 1998

Chemical Applications of Molecular Modelling Jonathan M. Goodman, 1998 This book explores the molecular modeling enabling the nonspecialist to appreciate the power as well as the limitations of the computational tools available and giving a background to the methods used and how they were developed It also provides examples of how molecular modeling has been used to address chemical questions commonly asked by the experimental chemist and includes practical examples and case studies 143 illus

Molecular Modeling of Crystallization from Solution Chengxiang Liu, 2018

D-Xylitol Silvio Silvério da Silva, Anuj Kumar Chandel, 2012-10-02 Commercially D xylitol is produced by chemical reactions that are tailored to the requirements of various sectors However due to the rising interest in sustainable development and ecologically benign practices microbial

transformation processes are generally preferred over the conventional chemical conversion process. The former have multiple advantages including less chemical load on the environment, higher efficiency, and the ability to dilute multiple downstream transformation attempts while maintaining product yield and recovery. This book aims to disseminate the most current advances in the biotechnological production of D xylitol and its applications in medical and health care. It is a unique collection of 15 book chapters split into 5 sections and written by experts in their respective fields who present critical insights into several topics, review current research, and discuss future progress in this area. This book also provides essential information on hemicellulose hydrolysis to recover D xylose, detoxification of hemicellulose hydrolysates, and improved fermentation methods for increased D xylitol production. The highlights of strain improvement to increase the D xylitol titers and downstream recovery of D xylitol are also discussed in several sections. The current applications of D xylitol in medical and health care have been used to justify the cost incurred for setting up the demonstration plant for D xylitol production in the market. Apart from researchers and post graduate students in the field of microbial biotechnology, this book will assist those in the business community who deal with the economic analysis of bio based products and their marketing.

Intrinsic Structures and Properties of Energetic Materials Chaoyang Zhang, Jing Huang, Rupeng Bu, 2023-06-30. This book highlights the intrinsic structures of all kinds of energetic compounds and some structure-property relationships therein. Energetic materials are a class of energy materials that can transiently release a large amount of gases and heat by self-redox after stimulated and usually refer to explosives, propellants, and pyrotechnics. Nowadays, in combination with various theories and simulation-aided material design technologies, many new kinds of energetic materials like energetic extended solids, energetic ionic salts, energetic metal-organic frameworks, energetic co-crystals, and energetic perovskites have been created in addition to traditional energetic molecular crystals. It is somewhat dazzling, and an issue of how we can understand these new types of energetic materials is raised. In the past about 20 years, we were immersed in the computational energetic materials. By means of defining a concept of intrinsic structures of energetic materials, which refers to the crystal packing structure of energetic materials as well as molecule-for-molecule solid, especially the microscopic structures, have been mostly clarified and related with many macroscopic properties and performances with molecular simulations. This book presents our understanding about it. Thereby, a simple and new way to readily understand energetic materials is expected to be paved based on this book. It contains energetic molecular crystals, energetic ionic crystals, energetic atomic crystals, energetic metallic crystals, and energetic mixed-type crystals, and the substructures closest to crystal packing. Meanwhile, the common intermolecular interactions in energetic crystals will be introduced. In addition, theoretical and simulation methods for treating the intrinsic structures will be briefed as they are the main tools to reveal the molecules and crystals. Besides the polymorphism as a level of intrinsic structures will be briefly discussed. In the final of this book, we introduce the crystal engineering of energetic materials. This book features the first proposal of intrinsic structure and crystal engineering of

energetic materials and the understanding of the properties and performances of energetic materials by maintaining a concept that structure determines property It helps to promote the rationality in creating new energetic materials rather than increase experience **Forthcoming Books** Rose Arny,1999 *Chemistry and Industry*,2000 Handbook of Polymer Crystallization Ewa Piorkowska,Gregory C. Rutledge,2013-07-01 Polymeric crystals are more complex in nature than other materials crystal structures due to significant structural disorder present The only comprehensive reference on polymer crystallization Handbook of Polymer Crystallization provides readers with a broad in depth guide on the subject covering the numerous problems encountered during crystallization as well as solutions to resolve those problems to achieve the desired result Edited by leading authorities in the field topics explored include neat polymers heterogeneous systems polymer blends polymer composites orientation induced crystallization crystallization in nanocomposites and crystallization in complex thermal processing conditions **Encyclopedia of Separation Science** Michael Cooke,C. F. Poole,2000

Relationship Between Crystal Structure and Solid-state Properties of Pharmaceuticals Agam R. Sheth,2004 *Molecular Modeling of Polymer Crystallization and the Effect of Nucleating Agents* Alexander Jules Bourque,2017 The microstructure in a semicrystalline polymer material ultimately determines its material properties Despite the abundance of research into the semicrystalline microstructure and its evolution during crystallization a clear description of its development remains elusive The advent of advanced computing and algorithms however have promoted molecular modeling of polymer crystallization providing a new perspective on the development of the microstructure This thesis revisits and challenges many aspects of microstructural development in macromolecular materials by applying new modeling techniques and recent technologies Through atomistic simulations of n alkane crystallization this thesis presents new molecular evidence of surface nucleation processes that contribute to the propagation of the crystal growth front in a macromolecular system Crystallization in polymeric systems has long been theorized to proceed by secondary nucleation In this work molecular dynamics MD simulations were engineered to probe this surface nucleation process by systematically inducing crystal growth for a system of macromolecules In a novel application of mean first passage time analysis the critical surface nucleus sizes waiting times and surface nucleation rates were extracted from atomically detailed molecular trajectories using a layer by layer approach Insight from MD simulations was used to build a new kinetic model to describe the structure and rate of advancement of the growth front during crystallization In the model solidification occurs through the mechanisms of surface nucleation and lateral spreading of the solid phase within layers in the vicinity of the growth front Transformation within each layer is described by an equation similar to the two dimensional variant of the Johnson Mehl Avrami equation The kinetic model is computationally efficient and predictive of important macroscopic observables Finally this thesis presents the first computational screening of nucleating agents for macromolecular crystallization Screens were conducted for two families of crystal materials tetrahedrally coordinated materials isomorphous to diamond and silicon and 2D hexagonally coordinated

materials isomorphic to graphene The induction time for heterogeneous nucleation was shown to depend strongly on crystallographic registry between the nucleating agent and the critical nucleus but the severity of this registry requirement weakened with increasing strength of attraction to the surface of the nucleating agent In an unprecedented find the substrate rigidity significantly influenced heterogeneous nucleation The molecular organization of nalkane chains at the nucleating surface was also investigated to build a fundamental understanding of the mechanisms for heterogeneous nucleation and spreading Modeling and Molecular Dynamics Simulation of Amorphous Silicon Crystallization Enrique Leal Jaen,2000 **Molecular Modeling of Inorganic Compounds** Peter Comba,Trevor W. Hambley,1995-09-13 An introduction to the field of molecular modelling of inorganic compounds which should be of interest to medicinal inorganic coordination and theoretical chemists The book provides reliable calculations of stereo selective interactions of metal complexes with biomolecules

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