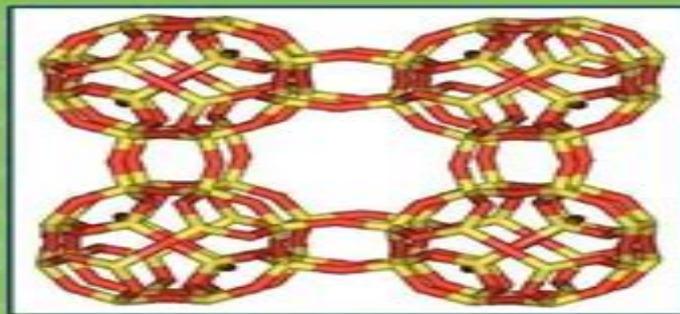




COMPUTER MODELLING OF MICROPOROUS MATERIALS

Edited by
C.R.A. CATLOW, R.A. VAN SANTEN & B. SMIT



Computer Modelling Of Microporous Materials

William Graham Richards



Computer Modelling Of Microporous Materials:

Computer Modelling of Microporous Materials C.Richard A. Catlow,Berend Smit,R.A. van Santen,2004-04-30

Microporous materials including both zeolites and aluminophosphates are amongst the most fascinating classes of materials with wide ranging important applications in catalysis gas separation and ion exchange The breadth of the field has moreover been extended in the last ten years by the discovery of the versatile and exciting ranges of mesoporous materials

Computational methods have a long and successful history of application in solid state and materials science where they are indeed established tools in modelling structural and dynamic properties of the bulk and surfaces of solids and where they are playing an increasingly important role in understanding reactivity Their application to zeolite science developed strongly in the 1980 s with the initial successes in modelling structure and sorption and with emerging capability in quantum mechanical methods The field was reviewed over ten years since then there have been major developments in techniques and of course the power of the available hardware which have promoted a whole range of new applications to real complex problems in the science of microporous materials Computer Modelling of Microporous Materials aims to summarise and illustrate the current capabilities of atomistic computer modelling methods in this growing field Details advances in the rapidly expanding field of microporous materials Summarises key current techniques in this type of modelling Illustrates the current capabilities of atomistic computer modelling methods

[Computer Modelling of Microporous and Mesoporous Materials](#) Charles Richard

Arthur Catlow,2004 Full text engineering e book **Computer Simulation of Porous Materials** Kim Jelfs,2021-08-31

Computer Simulation of Porous Materials covers the key approaches in the modelling of porous materials with a focus on how these can be used for structure prediction and to either rationalise or predict a range of properties including sorption diffusion mechanical spectroscopic and catalytic The book covers the full breadth of micro porous materials from inorganic zeolites to organic including porous polymers and porous molecular materials and hybrid materials metal organic frameworks Through chapters focusing on techniques for specific types of applications and properties the book outlines the challenges and opportunities in applying approaches and methods to different classes of systems including a discussion of high throughput screening There is a strong forward looking focus to identify where increased computer power or artificial intelligence techniques such as machine learning have the potential to open up new avenues of research Edited by a world leader in the field this title provides a valuable resource for not only computational researchers but also gives an overview for experimental researchers It is presented at a level accessible to advanced undergraduates postgraduates and researchers wishing to learn more about the topic

[Computer Modeling in Inorganic Crystallography](#) C.Richard A. Catlow,1997-02-03

Computer simulation techniques are now having a major impact on almost all areas of the physical and biological sciences This book concentrates on the application of these methods to inorganic materials including topical and industrially relevant systems including zeolites and high Tc superconductors The central theme of the book is the use of modern simulation

techniques as a structural tool in solid state science Computer Modelling in Inorganic Crystallography describes the current range of techniques used in modeling crystal structures and strong emphasis is given to the use of modeling in predicting new crystal structures and refining partially known structures It also reviews new opportunities being opened up by electronic structure calculation and explains the ways in which these techniques are illuminating our knowledge of bonding in solids Includes a thorough review of the technical basis of relevant contemporary methodologies including minimization Monte Carlo molecular dynamics simulated annealing methods and electronic structure methods Highlights applications to amorphous and crystalline solids Surveys simulations of surface and defect properties of solids Discusses applications to molecular and inorganic solids

Computer Modelling of Electronic and Atomic Processes in Solids Roderick Clarence Tennyson, Arnold E. Kiv, 1996-12-31 Thirty two proceedings papers from the May 1996 conference bringing together Eastern and Western scientists doing research in the areas of atomic and molecular processes electronic structure and processes and structure and properties The presentations focus on computer models ranging from fundamental atomic molecular and electronic structures and processes though macroscopic description of materials including discussions of environmental effects predictions of properties correlations with experiments and applications to space and electronics Additionally several featured presentations developed topics in fundamental theoretical models in materials science molecular dynamics simulations and an analysis of radiation processes in high temperature superconductor structures based on computer simulations Includes an appendix of workshop lectures and illustrations Annotation copyrighted by Book News Inc Portland OR

Chemistry of Zeolites and Related Porous Materials Ruren Xu, Wenqin Pang, Jihong Yu, Qisheng Huo, Jiasheng Chen, 2009-05-29 Widely used in adsorption catalysis and ion exchange the family of molecular sieves such as zeolites has been greatly extended and many advances have recently been achieved in the field of molecular sieves synthesis and related porous materials Chemistry of Zeolites and Related Porous Materials focuses on the synthetic and structural chemistry of the major types of molecular sieves It offers a systematic introduction to and an in depth discussion of microporous mesoporous and macroporous materials and also includes metal organic frameworks Provides focused coverage of the key aspects of molecular sieves Features two frontier subjects molecular engineering and host guest advanced materials Comprehensively covers both theory and application with particular emphasis on industrial uses This book is essential reading for researches in the chemical and materials industries and research institutions The book is also indispensable for researches and engineers in R D for catalysis divisions of companies in petroleum refining and the petrochemical and fine chemical industries

Catalytic Activation and Functionalisation of Light Alkanes E.G. Derouane, Jerzy Haber, Francisco Lemos, Fernando Ramôa Ribeiro, Michel Guisnet, 2013-11-11 Light alkanes tend to be resistant to many forms of activation The horizontal approach of the present book covers homogeneous heterogeneous and biological catalysis thus allowing readers to gain an awareness of progress and ideas in research areas different from their

own The book contains both general chapters giving an overview of the subject and specialised contributions that deal with the details and state of the art A specialist report is also included which gives a critical insight into current progress and discusses future prospects and major challenges Audience Newcomers and senior researchers in the field of alkane activation The mixed theoretical and practical approach will be of interest to researchers and industrialists alike

Computational Materials Science Charles Richard Arthur Catlow, Evgenii Alekseevich Kotomin, 2003 *Role of Interfaces in Environmental Protection* Sandor Barany, 2012-12-06 The NATO Advanced Research Workshop Role of Interfaces in Environmental Protection has been held on May 27 30 2002 in Miskolc Hungary under leadership of co directors Prof Sandor Barany from the University of Miskolc Hungary and Prof Nataliya Klymenko National Academy of Sciences of Ukraine The objective of the ARW was to highlight colloidal and biocolloidal aspects of environmental pollution and technologies to monitor remediate abate and prevent pollution It is known that the solution of majority of environmental problems is closely connected with phenomena at the interfaces The behaviour transport of dispersed particles in the environment the main phase separation methods in water treatment purification of liquids aerosols removal many soil remediation processes as well as the methods of protection of human organisms from hazardous matters are based on concepts of colloid chemistry i e properties of interfaces and their behaviour in different media Examples of these methods are filtration ultrafiltration flotation coagulation hetero coagulation and flocculation adsorption adhesion of micro organisms to surfaces membrane separation methods etc A very important and special aspect of the topic is the human protection using colloid chemical approaches i e the adsorption aggregation and adagulation properties of differe t materials Examples are adsorption of hazardous organic materials drugs heavy metals and radionuclides on activated carbon silica cellulose derivatives etc *Computer Modeling Studies of the Interstitial Structure of Selected Silica Polymorphs* Lilian Patricia Davila, 1998 *Faraday Discussions of the Chemical Society*, 1997 **Computer-aided Molecular Design** William Graham Richards, 1989 **Chemical Abstracts**, 2002 **Current Research in Britain**, 1991 *Proceedings from the Ninth International Zeolite Conference, Montreal, 1992* Roland von Ballmoos, John B. Higgins, Michael M. J. Treacy, 1992

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Modeling NMR Chemical Shifts Julio C. Facelli, 1999 This book reviews the history of NMR chemical shielding while surveying new developments in the field Topics include new methods for calculating NMR chemical shifts calculations of chemical shifts for important biological molecules new theories about the role of chemical shifts and modeling methods for chemical shifts in inorganic compounds **Powtech '83, Particle Technology** Institution of Chemical Engineers (Great

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