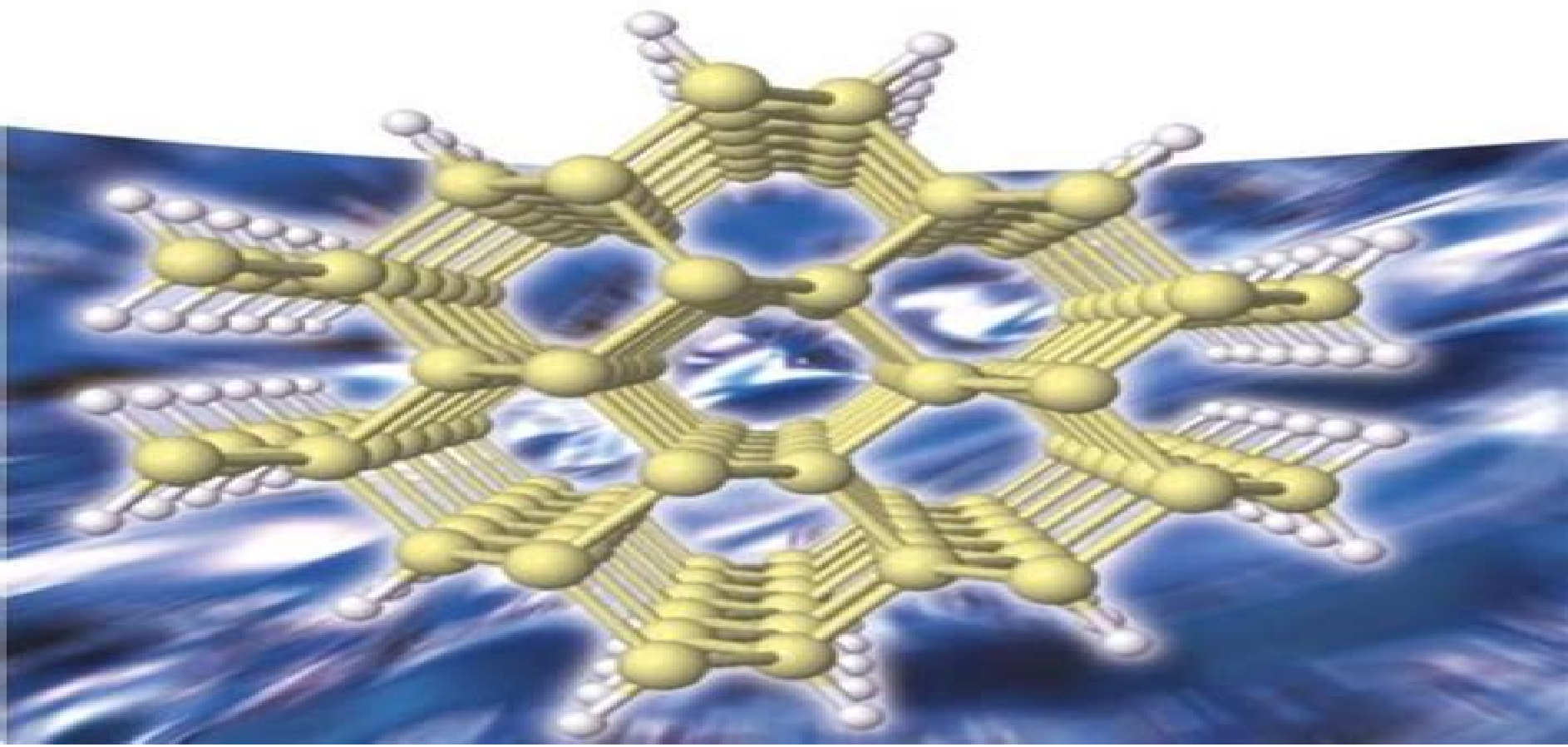


C. V. Ciobanu, C.-Z. Wang, and K.-M. Ho

Atomic Structure Prediction of Nanostructures, Clusters and Surfaces



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**Kristof T. Schütt, Stefan Chmiela, O.
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Müller**

Atomic Structure Prediction Of Nanostructures Clusters And Surfaces:

Atomic Structure Prediction of Nanostructures, Clusters and Surfaces Cristian V. Ciobanu, Cai-Zhuan Wang, Kai-Ming Ho, 2013-02-14 This work fills the gap for a comprehensive reference conveying the developments in global optimization of atomic structures using genetic algorithms Over the last few decades such algorithms based on mimicking the processes of natural evolution have made their way from computer science disciplines to solid states physics and chemistry where they have demonstrated their versatility and predictive power for many materials Following an introduction and historical perspective the text moves on to provide an in depth description of the algorithm before describing its applications to crystal structure prediction atomic clusters surface and interface reconstructions and quasi one dimensional nanostructures The final chapters provide a brief account of other methods for atomic structure optimization and perspectives on the future of the field

Superatoms Puru Jena, Qiang Sun, 2021-12-01 Explore the theory and applications of superatomic clusters and cluster assembled materials *Superatoms Principles Synthesis and Applications* delivers an insightful and exciting exploration of an emerging subfield in cluster science superatomic clusters and cluster assembled materials The book presents discussions of the fundamentals of superatom chemistry and their application in catalysis energy materials science and biomedical sciences Readers will discover the foundational significance of superatoms in science and technology and learn how they can serve as the building blocks of tailored materials promising to usher in a new era in materials science The book covers topics as varied as the thermal and thermoelectric properties of cluster based materials and clusters for CO₂ activation and conversion before concluding with an incisive discussion of trends and directions likely to dominate the subject of superatoms in the coming years Readers will also benefit from the inclusion of A thorough introduction to the rational design of superatoms using electron counting rules Explorations of superhalogens endohedrally doped superatoms and assemblies and magnetic superatoms A practical discussion of atomically precise synthesis of chemically modified superatoms A concise treatment of superatoms as the building blocks of 2D materials as well as superatom based ferroelectrics and cluster based materials for energy harvesting and storage Perfect for academic researchers and industrial scientists working in cluster science energy materials thermoelectrics 2D materials and CO₂ conversion *Superatoms Principles Synthesis and Applications* will also earn a place in the libraries of interested professionals in chemistry physics materials science and nanoscience

Advanced Topics in Contemporary Physics for Engineering Rui F. M. Lobo, Mário J. Pinheiro, 2022-12-21 This book highlights cutting edge topics in contemporary physics discussing exciting advances and new forms of thinking in evolving fields with emphases both on natural phenomena and applications to modern engineering It provides material for thought and practice in nanophysics plasma physics and electrodynamics Nanophysics and plasmas are synergic physical areas where the whole is more than the sum of the parts quantum atomic and molecular electrodynamics photonics condensed matter thermodynamics transport phenomena The authors emphasize both fundamentals and more

complex concepts making the contents accessible as well challenging Nanoscale properties and physical phenomena are explained under the umbrella of quantum physics Advances made in the physical knowledge of the nanoworld and its metrology are addressed along with experimental achievements which have furthered studies of extreme weak forces present at nano or sub micron scales The book does not focus in detail on the diversity of applications in nanotechnology and instrumentation considering that the reader already has basic prior knowledge on that It also covers an introduction to plasma universe phenomenology the basics of advanced mathematics applied to the electromagnetic field longitudinal forces in the vacuum concepts of helicity and topological torsion SU 2 representation of Maxwell equations 2D representation of the electromagnetic field the use of the fractional derivative and ergotropic dynamics The chapters include theory applications bibliographic references and solved exercises The synergies of the book s topics demonstrate their potential in critical issues such as relieving humans from barriers imposed by energetic and entropic dependencies and penetrating the realm of weak forces at the nanoscale The book will boost both post graduate students and mature scientists to implement new scientific and technological projects

Soft Computing in Chemical and Physical Sciences Kanchan Sarkar,Sankar Prasad Bhattacharyya,2017-11-06 This book can be regarded as Soft computing for physicists and chemists self taught It prepares the readers with a solid background of soft computing and how to adapt soft computing techniques to problem solving in physical and chemical research Soft computing methods have been little explored by researchers in physical and chemical sciences primarily because of the absence of books that bridge the gap between the traditional computing paradigm pursued by researchers in science and the new soft computing paradigm that has emerged in computer science This book is the interface between these primary sources and researchers in physics and chemistry

Handbook of Mechanical Nanostructuring Mahmood Aliofkhazraei,2016-05-02 Providing in depth information on how to obtain high performance materials by controlling their nanostructures this ready reference covers both the bottom up and the top down approaches to the synthesis and processing of nanostructured materials The focus is on advanced methods of mechanical nanostructuring such as severe plastic deformation including high pressure torsion equal channel angular processing cyclic extrusion compression accumulative roll bonding and surface mechanical attrition treatment As such the contents are inherently application oriented with the methods presented able to be easily integrated into existing production processes In addition the structure property relationships and ways of influencing the nanostructure in order to exhibit a desired functionality are reviewed in detail The whole is rounded off by a look at future directions followed by an overview of applications in various fields of structural and mechanical engineering With its solutions for successful processing of complex shaped workpieces and large scale specimens with desired properties this is an indispensable tool for purposeful materials design

Machine Learning Meets Quantum Physics Kristof T. Schütt,Stefan Chmiela,O. Anatole von Lilienfeld,Alexandre Tkatchenko,Koji Tsuda,Klaus-Robert Müller,2020-06-03 Designing molecules and materials with desired properties is an important

prerequisite for advancing technology in our modern societies This requires both the ability to calculate accurate microscopic properties such as energies forces and electrostatic multipoles of specific configurations as well as efficient sampling of potential energy surfaces to obtain corresponding macroscopic properties Tools that can provide this are accurate first principles calculations rooted in quantum mechanics and statistical mechanics respectively Unfortunately they come at a high computational cost that prohibits calculations for large systems and long time scales thus presenting a severe bottleneck both for searching the vast chemical compound space and the stupendously many dynamical configurations that a molecule can assume To overcome this challenge recently there have been increased efforts to accelerate quantum simulations with machine learning ML This emerging interdisciplinary community encompasses chemists material scientists physicists mathematicians and computer scientists joining forces to contribute to the exciting hot topic of progressing machine learning and AI for molecules and materials The book that has emerged from a series of workshops provides a snapshot of this rapidly developing field It contains tutorial material explaining the relevant foundations needed in chemistry physics as well as machine learning to give an easy starting point for interested readers In addition a number of research papers defining the current state of the art are included The book has five parts Fundamentals Incorporating Prior Knowledge Deep Learning of Atomistic Representations Atomistic Simulations and Discovery and Design each prefaced by editorial commentary that puts the respective parts into a broader scientific context

Atoms, Molecules and Clusters in Electric Fields George Maroulis, 2006 With the central importance of electric polarizability and hyperpolarizability for a wide spectrum of activities this book charts the trends in the accurate theoretical determination of these properties in specialized fields The contributions include reviews and original papers that extend from methodology to applications in specific areas of primary importance such as cluster science and organic synthesis of molecules with specific properties

In-vitro Materials Design Roman Leitsmann, Philipp Plänitz, Michael Schreiber, 2015-04-29 An overview of the latest computational materials science methods on an atomic scale The authors present the physical and mathematical background in sufficient detail for this highly current and important topic but without unnecessary complications They focus on approaches with industrial relevance covering real life applications taken from concrete projects that range from tribology modeling to performance optimization of integrated circuits Following an introduction to the fundamentals the book describes the most relevant approaches covering such classical simulation methods as simple and reactive force field methods as well as highly accurate quantum mechanical methods ranging from density functional theory to Hartree Fock and beyond A review of the increasingly important multiscale approaches rounds off this section The last section demonstrates and illustrates the capabilities of the methods previously described using recent real life examples of industrial applications As a result readers gain a heightened user awareness since the authors clearly state the conditions of applicability for the respective modeling methods so as to avoid fatal mistakes

Bimetallic Nanostructures Ya-Wen Zhang, 2018-08-06 Systematically summarizes

the current status and recent advances in bimetallic structures their shape controlled synthesis properties and applications Intensive researches are currently being carried out on bimetallic nanostructures focusing on a number of fundamental physical and chemical questions regarding their synthesis and properties This book presents a systematic and comprehensive summary of the current status and recent advances in this field supporting readers in the synthesis of model bimetallic nanoparticles and the exploration and interpretation of their properties Bimetallic Nanostructures Shape Controlled Synthesis for Catalysis Plasmonics and Sensing Applications is divided into three parts Part 1 introduces basic chemical and physical knowledge of bimetallic structures including fundamentals computational models and in situ characterization techniques Part 2 summarizes recent developments in synthetic methods characterization and properties of bimetallic structures from the perspective of morphology effect including zero dimensional nanomaterials one dimensional nanomaterials and two dimensional nanomaterials Part 3 discusses applications in electrocatalysis heterogeneous catalysis plasmonics and sensing Comprehensive reference for an important multidisciplinary research field Thoroughly summarizes the present state and latest developments in bimetallic structures Helps researchers find optimal synthetic methods and explore new phenomena in surface science and synthetic chemistry of bimetallic nanostructures Bimetallic Nanostructures Shape Controlled Synthesis for Catalysis Plasmonics and Sensing Applications is an excellent source or reference for researchers and advanced students Academic researchers in nanoscience nanocatalysis and surface plasmonics and those working in industry in areas involving nanotechnology catalysis and optoelectronics will find this book of interest

Technology and Innovation in Japan Martin Hemmert, Christian Oberländer, 1998-08-20 Long awaited reforms in technology policy and corporate strategy are now taking place in Japan This book asks whether it is the programme of reform or the will and ability to implement reforms which is new

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