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Carlo Gatti, Piero Macchi



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Modern Charge-Density Analysis Carlo Gatti, Piero Macchi, 2012-01-09 Modern Charge Density Analysis focuses on state of the art methods and applications of electron density analysis It is a field traditionally associated with understanding chemical bonding and the electrostatic properties of matter Recently it has also been related to predictions of properties and responses of materials having an organic inorganic or hybrid nature as in modern materials and bio science and used for functional devices or biomaterials Modern Charge Density Analysis is inherently multidisciplinary and written for chemists physicists crystallographers material scientists and biochemists alike It serves as a useful tool for scientists already working in the field by providing them with a unified view of the multifaceted charge density world Additionally this volume facilitates the understanding of scientists and PhD students planning to enter the field by acquainting them with the most significant and promising developments in this arena

Physics of Ferroelectrics Karin M. Rabe, Charles H. Ahn, Jean-Marc Triscone, 2007-07-20 During the past two decades revolutionary breakthroughs have occurred in the understanding of ferroelectric materials both from the perspective of theory and experiment First principles approaches including the Berry phase formulation of ferroelectricity now allow accurate quantitative predictions of material properties and single crystalline thin films are now available for fundamental studies of these materials In addition the need for high dielectric constant insulators and nonvolatile memories in semiconductor applications has motivated a renaissance in the investigation of these materials This book addresses the paradigmatic shifts in understanding brought about by these breakthroughs including the consideration of novel fabrication methods and nanoscale applications of these materials and new theoretical methods such as the effective Hamiltonian approach and density functional theory

Intelligent Computing Techniques for Smart Energy Systems Akhtar Kalam, Khaleequr Rehman Niazi, Amit Soni, Shahbaz Ahmed Siddiqui, Ankit Mundra, 2019-12-16 The book compiles the research works related to smart solutions concept in context to smart energy systems maintaining electrical grid discipline and resiliency computational collective intelligence consisted of interaction between smart devices smart environments and smart interactions as well as information technology support for such areas It includes high quality papers presented in the International Conference on Intelligent Computing Techniques for Smart Energy Systems organized by Manipal University Jaipur This book will motivate scholars to work in these areas The book also prophesies their approach to be used for the business and the humanitarian technology development as research proposal to various government organizations for funding approval

[The Quantum Theory of Atoms in Molecules](#) Chérif F. Matta, Russell J. Boyd, 2007-06-27 This book distills the knowledge gained from research into atoms in molecules over the last 10 years into a unique handy reference Throughout the authors address a wide audience such that this volume may equally be used as a textbook without compromising its research oriented character Clearly structured the text begins with advances in theory before moving on to theoretical studies of chemical bonding and reactivity There follow separate sections on solid state and

surfaces as well as experimental electron densities before finishing with applications in biological sciences and drug design. The result is a must have for physicochemists, chemists, physicists, spectroscopists and materials scientists.

Theoretical Modeling of Inorganic Nanostructures R.A. Evarestov, 2015-01-23. This book deals with the theoretical and computational simulation of monoperiodic nanostructures for different classes of inorganic substances. These simulations are related to their synthesis and experimental studies. A theoretical formalism is developed to describe 1D nanostructures with symmetric shapes and morphologies. Three types of models are considered for this aim: i) nanotubes rolled from 2D nanolayers and described within the formalism of line symmetry groups; ii) nanoribbons obtained from 2D nanolayers by their cutting along the chosen direction of translation; iii) nanowires obtained from 3D lattice by its sectioning along the crystalline planes parallel to the chosen direction of translation. Quantum chemistry ab initio methods applied for LCAO calculations on electronic and vibrational properties of 1D nanostructures are thoroughly described. Understanding of theoretical aspects presented here enlarges the possibilities for synthesis of monoperiodic nanostructures with predictable morphology and better interpretation of their properties.

High Performance Computing and Communications Ronald Perrott, 2007-09-17. This book constitutes the refereed proceedings of the Third International Conference on High Performance Computing and Communications (HPCC 2007) held in Houston, USA, September 26-28, 2007. The 75 revised full papers presented were carefully reviewed and selected from 272 submissions. The papers address all current issues of parallel and distributed systems and high performance computing and communication, as there are networking protocols, routing and algorithms, languages and compilers for HPC, parallel and distributed architectures and algorithms, embedded systems, wireless mobile and pervasive computing, Web services and internet computing, peer-to-peer computing, grid and cluster computing, reliability, fault tolerance and security, performance evaluation and measurement tools and environments for software development, distributed systems and applications, database applications and data mining, biological molecular computing, collaborative and cooperative environments and programming interfaces for parallel systems.

Grid Middleware and Services Domenico Talia, Ramin Yahyapour, Wolfgang Ziegler, 2008-06-07. Grid Middleware and Services: Challenges and Solutions is the eighth volume of the CoreGRID series. The CoreGrid Proceedings is the premiere European event on Grid Computing. This book aims to strengthen and advance scientific and technological excellence in the area of Grid Computing. The main focus in this volume is on Grid middleware and service level agreement. Grid middleware and Grid services are two pillars of grid computing systems and applications. This book includes high level contributions by leading researchers in both areas and presents current solutions together with future challenges. This volume includes sections on knowledge and data management on grids, Grid resource management and scheduling, Grid information resource and workflow monitoring services and service level agreements. Grid Middleware and Services: Challenges and Solutions is designed for a professional audience composed of researchers and practitioners in industry. This volume is also suitable for graduate level students in

computer science Applied Electromagnetism and Materials André Moliton, 2006-12-18 This book presents practical and relevant technological information about electromagnetic properties of materials and their applications. It is aimed at senior undergraduate and graduate students in materials science and is the product of many years of teaching basic and applied electromagnetism. Topics range from the spectroscopy and characterization of dielectrics to non-linear effects to ion beam applications in materials.

Advanced Solid-state Devices for Emerging Nanotechnologies Tarikul Islam, Shakeb Khan, Mohammad Khan, Monika Tomar, Shabana Mehfuz, 2025-09-12 Advanced Solid state Devices for Emerging Technologies provides a comprehensive overview of the transformative role played by nanotechnology in the development of solid state devices for various applications including efficient signal processing power data communication sensor and IoT enabled devices. The introductory section of the book provides the fundamental working principles of the solid state devices for signal processing energy harvesting and sensing of stimulants highlighting their significance for addressing some of the present challenges. The book also discusses the key structures of the devices with different functional units the role of basic and functionalized nanomaterials in enhancing their performance with diverse applications potential for sensing powering devices and signal processing. Other aspects covered include the experimental methods procedures in determining the response parameters of the devices and the application of artificial intelligence in modelling and optimization of system parameters. The proposed book is useful for researchers graduate students and undergraduate students working technical professionals in engineering and the sciences.

Key Features Discusses advanced materials and structures for developing emerging technologies for micro and nano applications Development of efficient interfacing and signal processing circuits with the idea of machine learning based sensor data and fault analysis Covers open research challenges and the future scope of research directions on emerging micro to nano technology

Journal of the Physical Society of Japan , 2013

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