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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

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

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