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Calculations on nonlinear optical properties for large systems Feng Long Gu, Yuriko Aoki, Michael Springborg, Bernard Kirtman, 2014-11-20 For design purposes one needs to relate the structure of proposed materials to their NLO nonlinear optical and other properties which is a situation where theoretical approaches can be very helpful in providing suggestions for candidate systems that subsequently can be synthesized and studied experimentally This brief describes the quantum mechanical treatment of the response to one or more external oscillating electric fields for molecular and macroscopic crystalline systems To calculate NLO properties of large systems a linear scaling generalized elongation method for the efficient and accurate calculation is introduced The reader should be aware that this treatment is particularly feasible for complicated three dimensional and or delocalized systems that are intractable when applied to conventional or other linear scaling methods

Physics of Quantum Rings Vladimir M. Fomin, 2013-08-29 This book deals with a new class of materials quantum rings Innovative recent advances in experimental and theoretical physics of quantum rings are based on the most advanced state of the art fabrication and characterization techniques as well as theoretical methods The experimental efforts allow to obtain a new class of semiconductor quantum rings formed by capping self organized quantum dots grown by molecular beam epitaxy Novel optical and magnetic properties of quantum rings are associated with non trivial topologies at the nanoscale An adequate characterization of quantum rings is possible on the basis of modern characterization methods of nanostructures such as Scanning Tunneling Microscopy A high level of complexity is demonstrated to be needed for a dedicated theoretical model to adequately represent the specific features of quantum rings The findings presented in this book contribute to develop low cost high performance electronic spintronic optoelectronic and information processing devices based on quantum rings

Quantum Mechanical/Molecular Mechanical Approaches for the Investigation of Chemical Systems - Recent Developments and Advanced Applications Thomas S. Hofer, Sam P. de Visser, 2018-11-28 The QM MM method short for quantum mechanical molecular mechanical is a highly versatile approach for the study of chemical phenomena combining the accuracy of quantum chemistry to describe the region of interest with the efficiency of molecular mechanical potentials to represent the remaining part of the system Originally conceived in the 1970s by the influential work of the the Nobel laureates Martin Karplus Michael Levitt and Arieh Warshel QM MM techniques have evolved into one of the most accurate and general approaches to investigate the properties of chemical systems via computational methods Whereas the first applications have been focused on studies of organic and biomolecular systems a large variety of QM MM implementations have been developed over the last decades extending the range of applicability to address research questions relevant for both solution and solid state chemistry as well Despite approaching their 50th anniversary in 2022 the formulation of improved QM MM methods is still an active field of research with the aim to i extend the applicability to address an even broader range of research questions in chemistry and related

disciplines and ii further push the accuracy achieved in the QM MM description beyond that of established formulations While being a highly successful approach on its own the combination of the QM MM strategy with other established theoretical techniques greatly extends the capabilities of the computational approaches For instance the integration of a suitable QM MM technique into the highly successful Monte Carlo and molecular dynamics simulation protocols enables the description of the chemical systems on the basis of an ensemble that is in part constructed on a quantum mechanical basis This eBook presents the contributions of a recent Research Topic published in Frontiers in Chemistry that highlight novel approaches as well as advanced applications of QM MM method to a broad variety of targets In total 2 review articles and 10 original research contributions from 48 authors are presented covering 12 different countries on four continents The range of research questions addressed by the individual contributions provide a lucid overview on the versatility of the QM MM method and demonstrate the general applicability and accuracy that can be achieved for different problems in chemical sciences Together with the development of improved algorithms to enhance the capabilities of quantum chemical methods and the continuous advancement in the capacities of computational resources it can be expected that the impact of QM MM methods in chemical sciences will be further increased already in the near future

The Encyclopedia of Physics Robert Martin Besançon, 1974 Concise signed articles most of them including bibliographic references on physics in general its major areas divisions and subdivisions as well as related topics such as astrophysics geophysics and biophysics Intended for physicists who need information outside their special field of interest librarians teachers engineers and other scientists who encounter physical concepts in pursuit of their profession Pref As a rule the technical level of the writing is higher for the more specialized areas than for the general topics Useful cross references Indexed Published 1974

Frontiers of Quantum Chemistry Marek J. Wójcik, Hiroshi Nakatsuji, Bernard Kirtman, Yukihiro Ozaki, 2017-11-06 The purpose of this book is to convey to the worldwide scientific community the rapid and enthusiastic progress of state of the art quantum chemistry Quantum chemistry continues to grow with remarkable success particularly due to rapid progress in supercomputers The usefulness of quantum chemistry is almost limitless Its application covers not only physical chemistry but also organic and inorganic chemistry physics and life sciences This book deals with all of these topics Frontiers of Quantum Chemistry is closely related to the symposium of the same name held at Kwansei Gakuin University at Nishinomiya Japan in November 2015 The book's contributors however include not only invited speakers at the symposium but also many other distinguished scientists from wide areas of quantum chemistry around the world

Progress in Computational Physics (PiCP): Volume 1 Matthias Ehrhardt, 2010 Progress in Computational Physics is a new e book series devoted to recent research trends in computational physics It contains chapters contributed by outstanding experts of modeling of physical problems The series focuses on interdisciplinary computat

Atomic Clusters with Unusual Structure, Bonding and Reactivity Pratim Kumar Chattaraj, Sudip Pan, Gabriel Merino, 2022-10-06 Atomic Clusters with Unusual Structure Bonding and Reactivity Theoretical

Approaches Computational Assessment and Applications reviews the latest computational tools and approaches available for accurately assessing the properties of a cluster while also highlighting how such clusters can be adapted and utilized for the development of novel materials and applications Sections provide an introduction to the computational methods used to obtain global minima for clusters and effectively analyze bonds outline experimental approaches to produce clusters discuss specific applications and explore cluster reactivity and usage across a number of fields Drawing on the knowledge of its expert editors and contributors this book provides a detailed guide to ascertaining the stability bonding and properties of atomic clusters Atomic clusters which exhibit unusual properties offer huge potential as building blocks for new materials and novel applications but understanding their properties stability and bonding is essential in order to accurately understand characterize and manipulate them for further use Searching for the most stable geometry of a given cluster is difficult and becomes even more so for clusters of medium and large sizes where the number of possible isomers sharply increase hence this book provides a unique and comprehensive approach to the topic and available techniques and applications Introduces readers to the vast structural and bonding diversity that clusters show and reflects on their potential for novel application and material development Highlights the latest computational methods and theoretical tools available for identification of the most stable isomers and accurate analysis of bonding in the clusters Focuses on clusters which violate the rules established in traditional chemistry and exhibit unusual structure bonding and reactivity

A Primer in Density Functional Theory
 Carlos Fiolhais, Fernando Nogueira, Miguel A.L. Marques, 2008-01-11 Density functional theory DFT is by now a well established method for tackling the quantum mechanics of many body systems Originally applied to compute properties of atoms and simple molecules DFT has quickly become a work horse for more complex applications in the chemical and materials sciences The present set of lectures spanning the whole range from basic principles to relativistic and time dependent extensions of the theory is the ideal introduction for graduate students or nonspecialist researchers wishing to familiarize themselves with both the basic and most advanced techniques in this field

Small Particles and Inorganic Clusters Claude Chapon, Marcel F. Gillet, Claude R. Henry, 2012-12-06 A lively demonstration of the great vitality and the multidisciplinary character of cluster research and of the usefulness of synthesizing its various aspects was given at this symposium This volume covers all aspects of the physical and chemical properties of free and supported clusters or small particles static dynamical electronic magnetic and optical properties adsorption and chemical phenomena It thus gives a complete overview of the status of the field and its development

Computational Multiscale Modeling of Fluids and Solids Martin Oliver Steinhauser, 2008 The idea of the book is to provide a comprehensive overview of computational physics methods and techniques that are used for materials modeling on different length and time scales Each chapter first provides an overview of the physical basic principles which are the basis for the numerical and mathematical modeling on the respective length scale The book includes the micro scale the meso scale and the macro scale The chapters follow this

classification The book will explain in detail many tricks of the trade of some of the most important methods and techniques that are used to simulate materials on the perspective levels of spatial and temporal resolution Case studies are occasionally included to further illustrate some methods or theoretical considerations Example applications for all techniques are provided some of which are from the author s own contributions to some of the research areas Methods are explained if possible on the basis of the original publications but also references to standard text books established in the various fields are mentioned

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