



Energetic Materials Part 1. Decomposition, Crystal and Molecular Properties

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eds.

Energetic Materials Pt 1 Decomposition Crystal And Molecular Properties

Suhithi M. Peiris, Gasper J. Piermarini



Energetic Materials Pt 1 Decomposition Crystal And Molecular Properties:

Energetic Materials ,2003-11-25 This volume provides an overview of current research and recent advances in the area of energetic materials focusing on decomposition crystal and molecular properties The contents and format reflect the fact that theory experiment and computation are closely linked in this field Since chemical decomposition is of fundamental importance in energetic performance this volume begins with a survey of the decomposition processes of a variety of energetic compounds This is followed by detailed studies of certain compounds and specific mechanisms such as nitro aci nitro tautomerism Chapter 6 covers the transition from decomposition to crystal properties with molecular dynamics being the primary analytical tool The next several chapters deal with different aspects of the crystalline state again moving from the general to particular There is also a discussion of methods for computing gas liquid and solid phase heats of formation Finally the last portion of this volume looks at the potential of high nitrogen molecules as energetic systems this has been of considerable interest in recent years Overall this volume illustrates the progress that has been made in the field of energetic materials and some of the areas of current activity It also indicates the challenges involved in characterizing and understanding the properties and behaviour of these compounds The work is a unique state of the art treatment of the subject written by pre eminent researchers in the field Overall emphasis is on theory and computation presented in the context of relevant experimental work Presents a unique state of the art treatment of the subject Contributors are preeminent researchers in the field

Molecular Modeling of the Sensitivities of Energetic Materials Didier Mathieu,2022-04-05 Molecular Modeling of the Sensitivities of Energetic Materials Volume 22 introduces experimental aspects explores the relationships between sensitivity molecular structure and crystal structure discusses insights from numerical simulations and highlights applications of these approaches to the design of new materials Providing practical guidelines for implementing predictive models and their application to the search for new compounds this book is an authoritative guide to an exciting field of research that warrants a computer aided approach for the investigation and design of safe and powerful explosives or propellants Much recent effort has been put into modeling sensitivities with most work focusing on impact sensitivity and leading to a lot of experimental data in this area Models must therefore be developed to allow evaluation of significant properties from the structure of constitutive molecules Highlights a range of approaches for computational simulation and the importance of combining them to accurately understand or estimate different parameters Provides an overview of experimental findings and knowledge in a quick and accessible format Presents guidelines to implement sensitivity models using open source python related software thus supporting easy implementation of flexible models and allowing fast assessment of hypotheses

Energetic Materials ,2003-11-21 This volume provides an overview of current research and recent advances in the area of energetic materials focusing on explosives and propellants The contents and format reflect the fact that theory experiment and computation are closely linked in this field The challenge of

developing energetic materials that are less sensitive to accidental stimuli continues to be of critical importance This volume opens with discussions of some determinants of sensitivity and its correlations with various molecular and crystal properties The next several chapters deal in considerable detail with different aspects and mechanisms of the initiation of detonation and its quantitative description The second half of this volume focuses upon combustion Extensive studies model ignition and combustion with applications to different propellants The final chapter is an exhaustive computational treatment of the mechanism and kinetics of combustion initiation reactions of ammonium perchlorate Overall this volume illustrates the progress that has been made in the field of energetic materials and some of the areas of current activity It also indicates the challenges involved in characterizing and understanding the properties and behaviour of these compounds The work is a unique state of the art treatment of the subject written by pre eminent researchers in the field Overall emphasis is on theory and computation presented in the context of relevant experimental work Presents a unique state of the art treatment of the subject Contributors are preeminent researchers in the field

The Properties of Energetic Materials Mohammad Hossein Keshavarz, Thomas M. Klapötke, 2017-11-20 For a chemist who is concerned with the synthesis of new energetic compounds it is essential to be able to assess physical and thermodynamic properties as well as the sensitivity of possible new energetic compounds before synthesis is attempted Various approaches have been developed to predict important aspects of the physical and thermodynamic properties of energetic materials including but not limited to crystal density heat of formation melting point enthalpy of fusion and enthalpy of sublimation of an organic energetic compound Since an organic energetic material consists of metastable molecules capable of undergoing very rapid and highly exothermic reactions many methods have been developed to estimate the sensitivity of an energetic compound with respect to detonation causing external stimuli such as heat friction impact shock and electrostatic discharge This book introduces these methods and demonstrates those methods which can be easily applied

Energetic Materials John R. Sabin, 2014-02-10 Advances in Quantum Chemistry presents surveys of current topics in this rapidly developing field that has emerged at the cross section of the historically established areas of mathematics physics chemistry and biology It features detailed reviews written by leading international researchers This volume focuses on the theory of heavy ion physics in medicine This volume presents a series of articles concerning current important topics in quantum chemistry The invited articles are written by the best people in the field

Static Compression of Energetic Materials Suhithi M. Peiris, Gasper J. Piermarini, 2009-01-03 Developing and testing novel energetic materials is an expanding branch of the materials sciences Reaction detonation or explosion of such materials invariably produce extremely high pressures and temperatures To study the equations of state EOS of energetic materials in extreme regimes both shock and static high pressure studies are required The present volume is an introduction and review of theoretical experimental and numerical aspects of static compression of such materials Chapter 1 introduces the basic experimental tool the diamond anvil pressure cell and the observational techniques used with it such as optical

microscopy infrared spectrometry and x ray diffraction Chapter 2 outlines the principles of high nitrogen energetic materials synthesis Chapters 3 and 4 examine and compare various EOS formalisms and data fitting for crystalline and non crystalline materials respectively Chapter 5 details the reaction kinetics of detonating energetic materials Chapter 6 investigates the interplay between static and dynamic shock studies Finally Chapters 7 and 8 introduce numerical simulations molecular dynamics of energetic materials under either hydrostatic or uni axial stress and ab initio treatments of defects in crystalline materials This timely volume meets the growing demand for a state of the art introduction and review of the most relevant aspects of static compression of energetic materials and will be a valuable reference to researchers and scientists working in academic industrial and governmental research laboratories

Properties and Functionalization of Graphene Dinadayalane Tandabany, Frank Hagelberg, 2022-05-10 *Properties and Functionalization of Graphene* Computational Chemistry Approaches Volume 21 shows how computational chemistry can be used to explore molecular interactions when modeling and manipulating graphene s properties for varied applications Sections compare results and experimental evidence cover the experimental techniques employed in the functionalization of graphene and associated challenges and delve into the properties of functionalized graphene Under the guidance of its expert editor this book shares insights from a global team of specialists making it an authoritative practical guide for all those studying developing or applying graphene across a whole range of fields Provides practical insights into the latest computational approaches used in modeling the properties of functionalized graphene Includes detailed methods and step by step guidance on key processes that are supported throughout with examples Highlights the electronic properties of functionalized graphene

Relativistic Electronic Structure Theory, 2004-03-05 The field of relativistic electronic structure theory is generally not part of theoretical chemistry education and is therefore not covered in most quantum chemistry textbooks This is due to the fact that only in the last two decades have we learned about the importance of relativistic effects in the chemistry of heavy and superheavy elements Developments in computer hardware together with sophisticated computer algorithms make it now possible to perform four component relativistic calculations for larger molecules Two component and scalar all electron relativistic schemes are also becoming part of standard ab initio and density functional program packages for molecules and the solid state The second volume of this two part book series is therefore devoted to applications in this area of quantum chemistry and physics of atoms molecules and the solid state Part 1 was devoted to fundamental aspects of relativistic electronic structure theory whereas Part 2 covers more of the applications side This volume opens with a section on the Chemistry of the Superheavy Elements and contains chapters dealing with Accurate Relativistic Fock Space Calculations for Many Electron Atoms Accurate Relativistic Calculations Including QED Parity Violation Effects in Molecules Accurate Determination of Electric Field Gradients for Heavy Atoms and Molecules Two Component Relativistic Effective Core Potential Calculations for Molecules Relativistic Ab Initio Model Potential Calculations for Molecules and Embedded Clusters

Relativistic Pseudopotential Calculations for Electronic Excited States Relativistic Effects on NMR Chemical Shifts Relativistic Density Functional Calculations on Small Molecules Quantum Chemistry with the Douglas Kroll Hess Approach to Relativistic Density Functional Theory and Relativistic Solid State Calculations Comprehensive publication which focuses on new developments in relativistic quantum electronic structure theory Many leaders from the field of theoretical chemistry have contributed to the TCC series Will no doubt become a standard text for scientists in this field **High Explosives, Propellants, Pyrotechnics** Ernst-Christian Koch, 2021-01-18 This dictionary contains 739 entries with about 1400 references to the primary literature Details on the composition performance sensitivity and other pertinent properties of Energetic Materials such as High Explosives Propellants Pyrotechnics as well as important ingredients such as Oxidizers Fuels Binders and Modifiers are given and presented partly in over 180 tables with more than 240 structural formulas In detail the dictionary gives elaborate descriptions of 460 Chemical Substances 170 Pyrotechnic Compositions 360 High Explosive and Propellant Formulations In addition the basic physical and thermochemical properties of 435 pure substances elements compounds typically occurring as ingredients or reaction products are given too 150 Figures schemes and diagrams explain Applications Test methods Scientific facilities and finally Individuals closely tied with the development and investigation of Energetic Materials The book is intended for readers with a technical or scientific background active in governmental agencies research institutes trade and industry concerned with the procurement development manufacture investigation and use of Energetic Materials such as High Explosives Propellants Pyrotechnics Fireworks and Ammunition The book serves both as a daily reference for the experienced as well as an introduction for the newcomer to the field

Python for Quantum Chemistry Qiming Sun, 2025-03-28 Quantum chemistry requires ever higher computational performance with more and more sophisticated and dedicated Python scripts being required to solve challenging problems Although resources for basic use of Python are widely and often freely available online and in literature truly cohesive materials for advanced Python programming skills are lacking Qiming Sun a developer of the popular Python package PySCF provides a comprehensive end to end practical resource for researchers and engineers who have basic Python programming experiences chiefly in computational chemistry but want to take their use of the software forwards to the next level the book provides an insightful exploration of Numpy Pandas and other data analysis tools Readers will learn how to manage their Python computational projects in a professional way with various tools and protocols for computational chemistry research and general scientific computing tasks exhibited and analysed from a technical perspective Multiple programming paradigms including object oriented functional meta programming dynamic concurrent and vector oriented are illustrated in various technology scenarios allowing readers to properly use them to enhance their program projects Readers will also learn how to use the presented optimization technologies to speed up their Python applications even to the level as fast as a native C implementation The applications of these technologies are then demonstrated using quantum chemistry Python applications

Python for Quantum Chemistry A Full Stack Programming Guide is written primarily for graduate students researchers and software engineers working primarily in the fields of theoretical chemistry computational chemistry condensed matter physics material modelling molecular simulations and quantum computing End to end guide for advanced Python programming skills and tools related to quantum chemistry research Tackles the following questions How can you ensure the Python runtime is manageable when the preliminary implementation becomes complicated or evolves many branches How do I ensure that others Python program works properly in my project How do I make my Python project reusable for others Covers in depth the crucial topic of Python code optimization methods with high performance computing technologies Provides examples of Python applications with cutting edge technologies such as automatic code generation cloud computing and GPGPU Includes discussion of Python runtime mechanism and advanced Python technologies *Chemistry of High-Energy Materials* Thomas M. Klapötke, 2015-11-13 Chemistry of High Energy Materials continues in this new and revised 3rd edition to provide fundamental scientific insights into primary and secondary explosives propellants rocket fuel and pyrotechnics The contents of the previous edition were meticulously updated and recent research developments added to this graduate level textbook Applications in military and civil fields are discussed Especially environmental issues caused by lead based primary explosives perchlorates in pyrotechnic formulations and modern signal flare compositions are discussed and current research presented Further additions include the understanding of the mechanism and continuing development of laser ignition methods techniques for the characterization of detonators and their output as well as principles and effects of underwater explosions New in the 3rd Edition Revised and updated content new study problems and questions Extended examination of the application of ionic liquids in the field and hydrodynamics Intended for advanced students in chemistry materials science and engineering as well as to all those working in defense technology This book makes a nice addition to the shelf of everyone involved with energetic materials As such it is recommended as a very useful reference for both students and experienced readers Ernst Christian Koch on the 2nd Edition in Propellants Explosive Pyrotechnics 16 2011 Upcoming titles by Thomas M Klap tke Energetic Materials Encyclopedia January 2018 Thomas M Klap tke CSci CChem FRSC was from 1995 until 1997 Ramsay Professor of Chemistry at the University of Glasgow in Scotland Since 1997 he has held the Chair of Inorganic Chemistry at LMU Munich **Prediction and Calculation of Crystal Structures** Sule Atahan-Evrenk, Alan Aspuru-Guzik, 2014-05-06 The series Topics in Current Chemistry presents critical reviews of the present and future trends in modern chemical research The scope of coverage is all areas of chemical science including the interfaces with related disciplines such as biology medicine and materials science The goal of each thematic volume is to give the non specialist reader whether in academia or industry a comprehensive insight into an area where new research is emerging which is of interest to a larger scientific audience Each review within the volume critically surveys one aspect of that topic and places it within the context of the volume as a whole The most significant developments of the last 5 to 10 years are

presented using selected examples to illustrate the principles discussed The coverage is not intended to be an exhaustive summary of the field or include large quantities of data but should rather be conceptual concentrating on the methodological thinking that will allow the non specialist reader to understand the information presented Contributions also offer an outlook on potential future developments in the field Review articles for the individual volumes are invited by the volume editors Readership research chemists at universities or in industry graduate students

Molecular and Nano Electronics: Analysis, Design and Simulation Jorge M. Seminario, 2006-10-24 The aim of Molecular and Nano Electronics Analysis Design and Simulation is to draw together contributions from some of the most active researchers in this new field in order to illustrate a theory guided approach to the design of molecular and nano electronics The field of molecular and nano electronics has driven solutions for a post microelectronics era where microelectronics dominate through the use of silicon as the preferred material and photo lithography as the fabrication technique to build binary devices transistors The construction of such devices yields gates that are able to perform Boolean operations and can be combined with computational systems capable of storing processing and transmitting digital signals encoded as electron currents and charges Since the invention of the integrated circuits microelectronics has reached increasing performances by decreasing strategically the size of its devices and systems an approach known as scaling down which simultaneously allow the devices to operate at higher speeds Provides a theory guided approach to the design of molecular and nano electronics Includes solutions for researchers working in this area Contributions from some of the most active researchers in the field of nano electronics

Theoretical Aspects of Chemical Reactivity, 2006-11-14 Theoretical Aspects of Chemical Reactivity provides a broad overview of recent theoretical and computational advancements in the field of chemical reactivity Contributions have been made by a number of leaders in the field covering theoretical developments to applications in molecular systems and clusters With an increase in the use of reactivity descriptors and fundamental theoretical aspects becoming more challenging this volume serves as an interesting overview where traditional concepts are revisited and explored from new viewpoints and new varieties of reactivity descriptors are proposed Includes applications in the frontiers of reactivity principles and introduces dynamic and statistical viewpoints to chemical reactivity and challenging traditional concepts such as aromaticity Written by specialists in the field of chemical reactivity An authoritative overview of the research and progress An essential reference material for students

Nitrogen-Rich Energetic Materials Michael Gozin, Leonid L. Fershtat, 2022-12-12 Nitrogen Rich Energetic Materials Provides in depth and comprehensive knowledge on both the chemistry and practical applications of nitrogen rich energetic materials Energetic materials a class of material with high amounts of stored chemical energy include explosives pyrotechnics and propellants Initially used for military applications nitrogen rich energetic materials have become important in the civil engineering and aerospace sectors they are increasingly used in commercial mining and construction as well as in rocket propulsion Making these nitrogen rich energetic materials safer more powerful and more cost effective

requires a thorough understanding of their chemistry physics synthesis properties and applications Nitrogen Rich Energetic Materials presents a detailed summary of the development of nitrogen rich energetic materials over the past decade and provides up to date knowledge on their applications in various areas of advanced engineering Edited by a panel of international experts in the field this book examines the chemistry of pentazoles fused ring and laser ignitable nitrogen rich compounds polynitrogen and tetrazole based energetic compounds and more The text also introduces applications of nitrogen rich energetic materials in energetic polymers and metal organic frameworks as pyrotechnics materials for light and smoke and in oxadiazoles from precursor molecules This authoritative volume Presents in depth chapters written by leading experts in each sub field covered Offers a systematic introduction to new and emerging applications of nitrogen rich energetic materials such as in computational chemistry Discusses recent advances in nitrate ester chemistry with focus on propellant applications Discusses green and eco friendly approaches to nitrogen rich compounds Nitrogen Rich Energetic Materials is an important resource for researchers academics and industry professionals across fields including explosives specialists pyrotechnicians materials scientists polymer chemists laser specialists physical chemists environmental chemists chemical engineers and safety officers High Energy Density Materials Thomas M. Klapötke, 2007-06-12

Nanomaterials: Design and Simulation Perla Balbuena, Jorge M. Seminario, 2006-11-02 Over the past few decades several approaches have been developed for designing nano structured or molecularly structured materials These advances have revolutionized practically all fields of science and engineering providing an additional design variable the feature size of the nano structures which can be tailored to provide new materials with very special characteristics Nanomaterials Design and Simulation explores the role that such advances have made toward a rational design of nanostructures and covers a variety of methods from ab initio electronic structure techniques ab initio molecular dynamics to classical molecular dynamics also being complemented by coarse graining and continuum methods Also included is an overview of how the development of these computational tools has enabled the possibility of exploring nanoscopic details and using such information for the prediction of physical and chemical properties that are not always possible to be obtained experimentally Provides an overview of approaches that have been developed for designing nano structured or molecularly structured materials This volume covers several aspects of the simulation and design of nanomaterials analyzed by a selected group of active researchers in the field Looks at how the advancement of computational tools have enabled nanoscopic prediction of physical and chemical properties *Computational Photochemistry* Massimo Olivucci, 2005-10-20 Computational Photochemistry Volume 16 provides an overview of general strategies currently used to investigate photochemical processes Whilst contributing to establishing a branch of computational chemistry that deals with the properties and reactivity of photoexcited molecules the book also provides insight into the conceptual and methodological research lines in computational photochemistry Packed with examples of applications of modelling of basic photochemical reactions and the

computer aided development of novel materials in the field of photodegradation paints photoprotection sunscreens color regulation photochromic devices and fluorescent probes this book is particularly useful to anyone interested in the effect of light on molecules and materials Provides an overview of computational photochemistry dealing with principles and applications Demonstrates techniques that can be used in the computer aided design of novel photo responsive materials Written by experts in computational photochemistry

The Crystalline States of Organic Compounds Angelo Gavezzotti, 2021-12-06 The Crystalline States of Organic Compounds is a broad survey of the techniques by which molecular crystals are investigated modeled and applied starting with the fundamentals of intra and intermolecular bonding supplemented by a concise tutorial on present day diffraction methods then proceeding to an examination of crystallographic databases with their statistics and of such fundamental and fast growing topics as intermolecular potentials polymorphism co crystallization and crystal structure prediction by computer A substantial part of the book is devoted to the techniques of choice in modern simulation Monte Carlo and molecular dynamics with their most recent developments and application to formed crystals and to the concomitant phases involved in nucleation and growth Drawing on the decades long experience of its author in teaching and research in the field of organic solid state The Crystalline States of Organic Compounds is an indispensable source of key insights and future directions for students and researchers at any level in academia and in industry Condenses theoretical information and practical methods in a single resource Provides a guide on the use of crystallographic databases structure statistics and molecular simulations Includes a large number of worked examples and tutorials with extensive graphics and multimedia

Computational Materials Science, 2004-03-19 Computational tools have been permanently deposited into the toolbox of theoretical chemists The impact of new computational tools can hardly be overestimated and their presence in research and applications is overwhelming Theoretical methods such as quantum mechanics molecular dynamics and statistical mechanics have been successfully used to characterize chemical systems and to design new materials drugs and chemicals This volume on Computational Material Sciences covers selected examples of notable applications of computational techniques to material science The chapters contained in this volume include discussions of the phenomenon of chaos in chemistry reaction network analysis and mechanisms of formation of clusters Details of more practical applications are also included in the form of reviews of computational design of new materials and the prediction of properties and structures of well known molecular assemblies Current developments of effective computational methods which will help in understanding predicting and optimizing periodic systems nanostructures clusters and model surfaces are also covered in this volume Reviews of current computational methods applied in material science Reviews of practical applications of modelling of structures and properties of materials Cluster and periodical approaches

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