Igor Samtsevich

Vladimir E. Fortov

Directory of Soviet Officials ,1983

National Library of Medicine Current Catalog National Library of Medicine (U.S.),1971 First multi-year cumulation covers six years: 1965-70.

Carbon in Earth Robert M. Hazen,Adrian P. Jones,John A. Baross,2018-12-17 Volume 75 of Reviews in Mineralogy and Geochemistry addresses a range of questions that were articulated in May 2008 at the First Deep Carbon Cycle Workshop in Washington, DC. At that meeting 110 scientists from a dozen countries set forth the state of knowledge about Earth's carbon. They also debated the key opportunities and top objectives facing the community. Subsequent deep carbon meetings in Bejing, China (2010), Novosibirsk, Russia (2011), and Washington, DC (2012), as well as more than a dozen smaller workshops, expanded and refined the DCO's decadal goals. The 20 chapters that follow elaborate on those opportunities and objectives.

National Union Catalog , Includes entries for maps and atlases.

Reactions at Solid Surfaces Gerhard Ertl,2010-06-17 Expanding on the ideas first presented in Gerhard Ertl's acclaimed Baker Lectures at Cornell University, Reactions at Solid Surfaces comprises an authoritative, self-contained, book-length introduction to surface reactions for both professional chemists and students alike. Outlining our present understanding of the fundamental processes underlying reactions at solid surfaces, the book provides the reader with a complete view of how chemistry works at surfaces, and how to understand and probe the dynamics of surface reactions. Comparing traditional surface probes with more modern ones, and bringing together various disciplines in a cohesive manner, Gerhard Ertl's Reactions at Solid Surfaces serves well as a primary text for graduate students in introductory surface science or chemistry, as well as a self-teaching resource for professionals in surface science,

chemical engineering, or nanoscience.

Carbon in Earth's Interior Craig E. Manning,Jung-Fu Lin,Wendy L. Mao,2020-04-03 Carbon in Earth's fluid envelopes - the atmosphere, biosphere, and hydrosphere, plays a fundamental role in our planet's climate system and a central role in biology, the environment, and the economy of earth system. The source and original quantity of carbon in our planet is uncertain, as are the identities and relative importance of early chemical processes associated with planetary differentiation. Numerous lines of evidence point to the early and continuing exchange of substantial carbon between Earth's surface and its interior, including diamonds, carbon-rich mantle-derived magmas, carbonate rocks in subduction zones and springs carrying deeply sourced carbon-bearing gases. Thus, there is little doubt that a substantial amount of carbon resides in our planet's interior. Yet, while we know it must be present, carbon's forms, transformations and movements at conditions relevant to the interiors of Earth and other planets remain uncertain and untapped. Volume highlights include: - Reviews key, general topics, such as carbonate minerals, the deep carbon cycle, and carbon in magmas or fluids - Describes new results at the frontiers of the field with presenting results on carbon in minerals, melts, and fluids at extreme conditions of planetary interiors - Brings together emerging insights into carbon's forms, transformations and movements through study of the dynamics, structure, stability and reactivity of carbon-based natural materials - Reviews emerging new insights into the properties of allied substances that carry carbon, into the rates of chemical and physical transformations, and into the complex interactions between moving fluids, magmas, and rocks to the interiors of Earth and other planets - Spans the various chemical redox states of carbon, from reduced hydrocarbons to zero-valent diamond and graphite to oxidized CO2 and carbonates - Captures and synthesizes the exciting results of recent, focused efforts in an

emerging scientific discipline - Reports advances over the last decade that have led to a major leap forward in our understanding of carbon science - Compiles the range of methods that can be tapped tap from the deep carbon community, which includes experimentalists, first principles theorists, thermodynamic modelers and geodynamicists - Represents a reference point for future deep carbon science research Carbon in Planetary Interiors will be a valuable resource for researchers and students who study the Earth's interior. The topics of this volume are interdisciplinary, and therefore will be useful to professionals from a wide variety of fields in the Earth Sciences, such as mineral physics, petrology, geochemistry, experimentalists, first principles theorists, thermodynamics, material science, chemistry, geophysics and geodynamics.

Theoretical Electrochemistry Lev Ivanovich Antropov,2001

Handbook of Solid State Chemistry, 6 Volume Set Richard Dronskowski,Shinichi Kikkawa,Andreas Stein,2017-10-23 This most comprehensive and unrivaled compendium in the field provides an up-to-date account of the chemistry of solids, nanoparticles and hybrid materials. Following a valuable introductory chapter reviewing important synthesis techniques, the handbook presents a series of contributions by about 150 international leading experts -- the Who's Who of solid state science. Clearly structured, in six volumes it collates the knowledge available on solid state chemistry, starting from the synthesis, and modern methods of structure determination. Understanding and measuring the physical properties of bulk solids and the theoretical basis of modern computational treatments of solids are given ample space, as are such modern trends as nanoparticles, surface properties and heterogeneous catalysis. Emphasis is placed throughout not only on the design and structure of solids but also on practical applications of these novel materials in real chemical situations.

Carbonates Richard J. Reeder,2018-12-17 Volume 11 of

Reviews in Mineralogy attempts to synthesize our present understanding of certain aspects of the mineralogy and chemistry of the rock-forming carbonates. This review follows, by ten years, a major assessment of (sedimentary) carbonate minerals by Lippmann (1973). There is only minor overlap of subject material, and I hope that this difference reflects fairly how this field has developed. In this volume, some of the papers are general (i.e., those addressing crystal chemistry and phase relations), and they provide overviews of a fundamental nature and are of interest to many. Others are more specialized in coverage and generally reflect the different approaches used in carbonate geochemistry. The final chapter introduces transmission electron microscopy, a relatively new and powerful technique for mineralogical research that has great potential in carbonate research.

Magmas Under Pressure Yoshio Kono,Chrystèle Sanloup,2018-04-06 Magmas under Pressure: Advances in High-Pressure Experiments on Structure and Properties of Melts summarizes recent advances in experimental technologies for studying magmas at high pressures. In the past decade, new developments in high-pressure experiments, particularly with synchrotron X-ray techniques, have advanced the study of magmas under pressure. These new experiments have revealed significant changes of structure and physical properties of magmas under pressure, which significantly improves our understanding of the behavior of magmas in the earth's interior. This book is an important reference, not only in the earth and planetary sciences, but also in other scientific fields, such as physics, chemistry, material sciences, engineering and in industrial applications, such as glass formation and metallurgical processing. Includes research and examples of high-pressure technologies for studying the structure and properties of magma Summarizes the current knowledge on the structure and properties of high-pressure magma Highlights the importance of magma in understanding the evolution of the earth's interior

Computational Materials Discovery Artem Oganov,Gabriele Saleh,Alexander Kvashnin,2018-10-30 New technologies are made possible by new materials, and until recently new materials could only be discovered experimentally. Recent advances in solving the crystal structure prediction problem means that the computational design of materials is now a reality. Computational Materials Discovery provides a comprehensive review of this field covering different computational methodologies as well as specific applications of materials design. The book starts by illustrating how and why first-principle calculations have gained importance in the process of materials discovery. The book is then split into three sections, the first exploring different approaches and ideas including crystal structure prediction from evolutionary approaches, data mining methods and applications of machine learning. Section two then looks at examples of designing specific functional materials with special technological relevance for example photovoltaic materials, superconducting materials, topological insulators and thermoelectric materials. The final section considers recent developments in creating low-dimensional materials. With contributions from pioneers and leaders in the field, this unique and timely book provides a convenient entry point for graduate students, researchers and industrial scientists on both the methodologies and applications of the computational design of materials.

The Physics of Non-ideal Plasma V. E. Fortov,Igor T. Iakubov,2000 &Quot;This book is devoted to the physical properties of non-ideal plasma which are compressed so strongly that the effects of interparticle interactions govern its behavior. In this volume, the methods of non-ideal plasma generation and diagnostics are considered. The experimental results are given and the main theoretical models of the non-ideal plasma state are discussed. The problems of thermodynamics, electro-physics, optics and dynamic stability are covered.--BOOK JACKET.

Extreme States of Matter Vladimir E. Fortov,2015-12-26 With its many beautiful colour pictures, this book gives fascinating insights into the unusual forms and behaviour of matter under extremely high pressures and temperatures. These extreme states are generated, among other things, by strong shock, detonation and electric explosion waves, dense laser beams, electron and ion beams, hypersonic entry of spacecraft into dense atmospheres of planets and in many other situations characterized by extremely high pressures and temperatures. Written by one of the world's foremost experts on the topic, this book will inform and fascinate all scientists dealing with materials properties and physics and also serve as an excellent introduction to plasma-, shock-wave and high-energy-density physics for students and newcomers seeking an overview. This second edition is thoroughly revised and expanded, in particular with new material on high energy-density physics, nuclear explosions and other nuclear transformation processes.

Lattice dynamics Johan Tidholm,2020-11-02 The reason to perform calculations in material science usually falls into one of two categories: to predict or explain the origin of material properties. This thesis covers first-principle calculations for solids at extreme conditions, from both of the two mentioned categories. I primarily have studied the effects of high-pressure and high-temperature on lattice dynamics, mechanical and electronic properties. To treat the effects of temperature, ab initio molecular dynamics (AIMD) simulations and self-consistent phonon calculations, based on density functional theory, have been utilised. These approaches account for the temperature effects by considering thermally excited supercells as samples of a statistical ensemble. To extract properties from this representation, I have used methods which maps the supercell data to a unit cell representation or fits it to a simple model Hamiltonian. The small displacement method was used to analyse the dynamical stability for nitrides and polymorphs of silica,

synthesised at high-pressure in a diamond anvil cell. The nitride compounds consist of a high amount of nitrogen either as chains, forming a porous framework together with transition metal atoms or as dinitrogen molecules, occupying the channels of the framework. The nitrogen chains consist of single- or double-bonded nitrogen atoms, making these compounds highly energetic. Polymorphs of silica can be used to model deep Earth liquids. These new polymorphs, named coesite-IV and coesite-V, consist of four-, five-, and six-oriented silicon. Some of the octahedra of the six-oriented silicon atoms, of these new phases, are sharing faces, which according to Pauling's third rule would make them highly unstable. My phonon calculations indicate these phases to be dynamically stable. Furthermore, my calculations predict higher compressibility for these new phases compared to the competing ones. By modelling silicate melts with coesite-IV and coesite-V, a more complex and compressible structure is expected, affecting the predicted seismic behaviour. I studied Kohn anomalies for body-centered cubic niobium by simulating this material with self-consistent phonon calculations. The electronic structure was studied by using a band unfolding technique, for which I obtained an effective unit cell representation of the electronic structure at elevated temperatures. Temperature primarily smeared the electronic states but did not induce significant shifts of the bands. In parallel, the anharmonicity of this system was studied using the temperature dependent effective potential method. Even close to the melting temperature, this element is remarkably harmonic. The experimentally observed disappearance of the Kohn anomalies with increased temperature is predominantly dependent, according to my calculations, on the temperature-induced smearing of the electronic states. Using stress-strain relations, accurate high-temperature elastic properties were predicted for Ti0.5Al0.5N. The simulations were performed with AIMD. The stresses were fitted using the least-squares method to

a linear expression from which the elastic constants were derived. The results were compared with previously performed calculations that employed additional approximations. The results of the symmetry imposed force constant temperature dependent effective potential (SIFC-TDEP) method agrees well with our results. I also compared my results with TiN calculations that employed a similar methodology. My and the SIFC-TDEP results are reporting lower values for the polycrystalline moduli than the calculations for TiN. The data I generated were also used for a machine learned interatomic potential method, where moment tensor potentials were trained and evaluated, using this data. Den här avhandlingen handlar om beräkningar för material. När materialberäkningar utförs är det antingen för att förutsäga eller förklara egenskaper. De beräkningar som jag har gjort i denna avhandling är baserade på fundamentala fysiska lagar. Detta betyder att de är rent baserade på teori, och inte har anpassats efter resultat av experiment. Jag har i mitt arbete använt mig mycket utav en teori som kallas gitter dynamik. Den är definierad för periodiska material, det vill säga att atomerna i dessa material upprepas i periodiska mönster. Vi kan då anta att det finns en jämviktspunkt för alla atomerna, som de vibrerar omkring. Dessa vibrationer kan beskrivas som om atomerna påverkar varandra med fiktiva fjädrar. Genom att beräkna styrkan för dessa fjädrar kan vi beskriva vibrationerna av atomerna. Dessa vibrationer i sin tur är avgörande för materialets egenskaper. För att beskriva ett material vid en specifik temperatur har jag använt mig utav olika metoder för att simulera det. En simulering kan ses som ett "dator experiment". Problemet är dock hur vi ska mäta egenskaperna i simuleringen. Ju större och mera komplex en simulering är, desto svårare blir det att beräkna egenskaperna av det simulerade materialet. Vi hamnar i en situation likt den vi skulle befinna oss om vi hade gjort ett experiment i verkligheten, och tvingas använda förenklade modeler för att kunna tolka resultatet. Jag har därför använt mig utav metoder för att utvinna

vibrationer av atomer, elektrontillstånd eller elastiska egenskaper, specifikt utvecklade för att användas på denna typ utav simuleringar. Mitt arbete har kretsat kring hur dessa egenskaper påverkas av extrema temperaturer och tryck. De beräkningar jag har utfört vid höga tryck har varit för nyupptäckta nitrider och faser av kiseldioxid. Nitriderna är porösa material som innehåller en stor mängd kväve. Det höga kväveinehållet gör så att det lagras en stor mängd kemisk energi i enkel- och dubbelbindningar mellan kväveatomerna. De nya faserna av kiseldioxid har en betydelse för vår förståelse av jordens inre. Deras existens öppnar upp för att det kan finnas mera komplexa och ihoptryckbara flytande material, under jordens nedre mantel, än vad tidigare har varit antaget. Mina beräkningar har bekräftat strukturerna för dessa nyupptäckta material. Vid höga temperaturer har jag studerat för metallen niob hur vibrationerna av atomerna är relaterade till olika elektrontillstånd. För specifika vibrationer ökar frekvensen med ökad temperatur. Detta är något ovanligt eftersom vibrationernas frekvenser vanligtvis brukar minska med ökad temperatur. Mina simulering för denna metal överensstämmer med resultat från experiment. Orsaken till varför visa vibrationers frekvenser ökar kan jag förklara med att elektrontillståndens enskilda energier varierar över tid på grund av den ökade temperaturen. Jag har även använt mig av simuleringar för att beräkna elastiska egenskaper av legeringen Ti0.5Al0.5N. Ti1?xAlxN legeringar används som beläggningar på skärverktyg som används för metall. För att öka effektiviteten av beläggningen, behövs det detaljerad kunskap av dess mekaniska egenskaper för den temperatur som de används vid. Jag beräknade därför så noggrant som möjligt de elastiska egenskaperna för Ti0.5Al0.5N. Dessa beräkningar är avsedda för att användas som en referens för andra beräkningsmässigt billigare metoder. Datan som genererades från mina simuleringar användes även för en sådan metod, baserad på maskininlärning.

Computational Catalysis Aravind Asthagiri,Michael Janik,2014 This book presents a comprehensive review of the methods and approaches being adopted to push forward the boundaries of computational catalysis.

First virtual Bilateral Conference on Functional Materials (BiC-FM) Scientific committee,

Heterogeneous Catalysts Wey Yang Teoh,Atsushi Urakawa,Yun Hau Ng,Patrick Sit,2021-02-23 Presents state-of-the-art knowledge of heterogeneous catalysts including new applications in energy and environmental fields This book focuses on emerging techniques in heterogeneous catalysis, from new methodology for catalysts design and synthesis, surface studies and operando spectroscopies, ab initio techniques, to critical catalytic systems as relevant to energy and the environment. It provides the vision of addressing the foreseeable knowledge gap unfilled by classical knowledge in the field. Heterogeneous Catalysts: Advanced Design, Characterization and Applications begins with an overview on the evolution in catalysts synthesis and introduces readers to facets engineering on catalysts; electrochemical synthesis of nanostructured catalytic thin films; and bandgap engineering of semiconductor photocatalysts. Next, it examines how we are gaining a more precise understanding of catalytic events and materials under working conditions. It covers bridging pressure gap in surface catalytic studies; tomography in catalysts design; and resolving catalyst performance at nanoscale via fluorescence microscopy. Quantum approaches to predicting molecular reactions on catalytic surfaces follows that, along with chapters on Density Functional Theory in heterogeneous catalysis; first principles simulation of electrified interfaces in electrochemistry; and high-throughput computational design of novel catalytic materials. The book also discusses embracing the energy and environmental challenges of the 21st century through heterogeneous catalysis and much more. Presents recent developments in heterogeneous catalysis with emphasis on new

fundamentals and emerging techniques Offers a comprehensive look at the important aspects of heterogeneous catalysis Provides an applications-oriented, bottoms-up approach to a high-interest subject that plays a vital role in industry and is widely applied in areas related to energy and environment Heterogeneous Catalysts: Advanced Design, Characterization and Applications is an important book for catalytic chemists, materials scientists, surface chemists, physical chemists, inorganic chemists, chemical engineers, and other professionals working in the chemical industry.

Directory of Soviet Officials ,1986

Chemical Complexity Alexander S. Mikhailov,Gerhard Ertl,2017-08-10 This book provides an outline of theoretical concepts and their experimental verification in studies of self-organization phenomena in chemical systems, as they emerged in the mid-20th century and have evolved since. Presenting essays on selected topics, it was prepared by authors who have made profound contributions to the field. Traditionally, physical chemistry has been concerned with interactions between atoms and molecules that produce a variety of equilibrium structures - or the 'dead' order - in a stationary state. But biological cells exhibit a different 'living' kind of order, prompting E. Schrödinger to pose his famous question “What is life?” in 1943. Through an unprecedented theoretical and experimental development, it was later revealed that biological self-organization phenomena are in complete agreement with the laws of physics, once they are applied to a special class of thermodynamically open systems and non-equilibrium states. This knowledge has in turn led to the design and synthesis of simple inorganic systems capable of self-organization effects. These artificial 'living organisms' are able to operate on macroscopic to microscopic scales, even down to single-molecule machines. In the future, such research could provide a basis for a technological breakthrough, comparable in its impact with the invention of lasers and semiconductors. Its

results can be used to control natural chemical processes, and to design artificial complex chemical processes with various functionalities. The book offers an extensive discussion of the history of research on complex chemical systems and its future prospects.

Theoretical and Computational Methods in Mineral Physics Renata M. Wentzcovitch,Lars Stixrude,2018-12-17 Volume 71 of Reviews in Mineralogy and Geochemistry represents an extensive review of the material presented by the invited speakers at a short course on Theoretical and Computational Methods in Mineral Physics held prior (December 10-12, 2009) to the Annual fall meeting of the American Geophysical Union in San Francisco, California. The meeting was held at the Doubletree Hotel & Executive Meeting Center in Berkeley, California. Contents: Density functional theory of electronic structure: a short course for mineralogists and geophysicists The Minnesota density functionals and their applications to problems in mineralogy and geochemistry Density-functional perturbation theory for quasi-harmonic calculations Thermodynamic properties and phase relations in mantle minerals investigated by first principles quasiharmonic theory First principles quasiharmonic thermoelasticity of mantle minerals An overview of quantum Monte Carlo methods Quantum Monte Carlo studies of transition metal oxides Accurate and efficient calculations on strongly correlated minerals with the LDA+U method: review and perspectives Spin-state crossover of iron in lower-mantle minerals: results of DFT+U investigations Simulating diffusion Modeling dislocations and plasticity of deep earth materials Theoretical methods for calculating the lattice thermal conductivity of minerals Evolutionary crystal structure prediction as a method for the discovery of minerals and materials Multi-Mbar phase transitions in minerals Computer simulations on phase transitions in ice Iron at Earth’s core conditions from first principles calculations First-principles

molecular dynamics simulations of silicate melts: structural and dynamical properties Lattice dynamics from force-fields as a technique for mineral physics An efficient cluster expansion method for binary solid solutions: application to the halite-silvite, NaCl-KCl, system Large scale simulations Thermodynamics of the Earth’s mantle

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