solid state chemistry and its applications

Solid State Chemistry and Its Applications: Exploring the Heart of Modern Materials

solid state chemistry and its applications form the backbone of many technological advancements that shape our daily lives. From the smartphone in your hand to the batteries powering electric vehicles, this fascinating branch of chemistry dives deep into the structure, properties, and transformations of solid materials. Unlike traditional chemistry, which often focuses on molecules in solution or gas phases, solid state chemistry investigates the intricate arrangements and interactions within solids—be they crystalline, amorphous, or somewhere in between. This article will take you on an engaging journey through the fundamentals of solid state chemistry and reveal how its applications influence everything from electronics to energy storage, catalysis, and even medicine.

Understanding the Basics of Solid State Chemistry

Solid state chemistry primarily deals with the study of the synthesis, structure, and properties of solid materials. It encompasses a wide range of substances, including metals, ceramics, semiconductors, and polymers. At its core, this field seeks to understand how atoms and ions are arranged in solids and how these arrangements affect physical and chemical properties.

The Role of Crystal Structures

One of the foundational concepts in solid state chemistry is crystal structure. Most solids are crystalline, meaning their atoms are arranged in highly ordered, repeating patterns. These patterns determine many material properties such as electrical conductivity, magnetism, hardness, and optical behavior.

For example, the difference between graphite and diamond—the two allotropes of carbon—lies entirely in their crystal structures. Graphite has layers of hexagonally arranged carbon atoms that slide over each other easily, making it soft and conductive. Diamond, on the other hand, has a rigid three-dimensional network of carbon atoms, resulting in unmatched hardness and optical brilliance.

Defects and Their Influence

No crystal is perfect; defects are intrinsic to solid materials. These imperfections, such as vacancies (missing atoms), interstitials (extra atoms squeezed in), and dislocations (misaligned planes), significantly influence the properties of materials. In fact, the

controlled introduction of defects (doping) is essential in developing semiconductors and other advanced materials.

Applications of Solid State Chemistry in Modern Technology

The practical applications of solid state chemistry are vast and impactful. By manipulating the atomic and molecular structure of solids, scientists and engineers create materials with tailored properties, enabling breakthroughs in numerous fields.

Electronics and Semiconductor Industry

Solid state chemistry is the cornerstone of semiconductor technology, which powers all modern electronics—from computers and smartphones to LED displays and solar cells. Understanding the crystal structure and electronic band structure of semiconductors like silicon, gallium arsenide, and perovskites allows engineers to optimize their electrical properties.

Doping semiconductors with specific impurities enables precise control over conductivity, creating p-type and n-type materials essential for diodes, transistors, and integrated circuits. Innovations in solid state chemistry have also led to the development of novel materials such as organic semiconductors and quantum dots, pushing the envelope of device performance.

Energy Storage and Batteries

The demand for efficient, safe, and long-lasting batteries has skyrocketed with the rise of portable electronics and electric vehicles. Solid state chemistry provides the foundation for the development of advanced battery materials, including lithium-ion, solid-state, and sodium-ion batteries.

For instance, the discovery and optimization of solid electrolytes—materials that conduct ions while being electronically insulating—are key to creating safer batteries that don't rely on flammable liquid electrolytes. Solid state electrolytes like garnet-type oxides and sulfides offer high ionic conductivity and chemical stability, promising longer battery life and enhanced safety.

Catalysis and Environmental Applications

Catalysts accelerate chemical reactions without being consumed, and many catalysts are solid materials with intricate surface structures. Solid state chemistry helps in designing catalysts with high surface area, optimal active sites, and stability under reaction

conditions.

Zeolites, a class of microporous aluminosilicate minerals, exemplify how solid state chemistry enables selective catalysis in petroleum refining and environmental cleanup. Their well-defined pore structures allow for molecular sieving and enhanced reaction control. Similarly, metal oxide catalysts are widely used for pollution control, such as in automotive catalytic converters that reduce harmful emissions.

Pharmaceuticals and Drug Delivery

While pharmaceuticals are often associated with molecular chemistry, solid state chemistry plays a crucial role in drug formulation and delivery. Many drugs exist in multiple solid forms—polymorphs, hydrates, or amorphous states—that affect their solubility, and bioavailability.

Understanding and controlling these solid forms can improve drug efficacy and shelf life. Moreover, solid state chemistry underpins the design of advanced drug delivery systems like controlled-release tablets and nanoparticle carriers, enhancing targeted therapy and patient compliance.

Emerging Trends and Future Directions

With rapid advances in instrumentation and computational methods, solid state chemistry continues to evolve, opening avenues for novel materials and applications.

Nanomaterials and Quantum Materials

At the nanoscale, materials exhibit unique properties that differ significantly from their bulk counterparts. Solid state chemistry is central to synthesizing and characterizing nanomaterials, which find applications in catalysis, electronics, and medicine.

Quantum materials—such as topological insulators and superconductors—are also at the forefront of research. Their exotic electronic properties stem from the quantum mechanical behavior of electrons in solid lattices, offering potential breakthroughs in quantum computing and spintronics.

Advanced Characterization Techniques

Modern solid state chemistry relies heavily on sophisticated analytical tools to unravel the structure and dynamics of solids. Techniques like X-ray diffraction (XRD), electron microscopy, nuclear magnetic resonance (NMR), and neutron scattering provide detailed insights into atomic arrangements and defects.

Complementing experiments, computational modeling using density functional theory (DFT) and molecular dynamics simulations enables scientists to predict material properties and guide synthesis.

Tips for Students and Researchers Diving into Solid State Chemistry

If you're intrigued by solid state chemistry and its applications, here are a few tips to deepen your understanding and skills:

- Master crystallography basics: Knowing how to interpret and analyze crystal structures is fundamental.
- **Get hands-on experience:** Laboratory work with synthesis and characterization techniques solidifies theoretical knowledge.
- **Stay updated with current research:** The field is dynamic; reading journals and attending seminars will keep you informed about breakthroughs.
- Leverage computational tools: Familiarize yourself with software for modeling and simulations to complement experimental work.
- **Collaborate across disciplines:** Solid state chemistry intersects with physics, materials science, and engineering, so interdisciplinary teamwork is valuable.

Exploring the world of solid state chemistry opens up a realm where atomic-scale understanding translates into tangible innovations. Whether it's developing the next-generation battery or designing smart materials for environmental solutions, the applications of solid state chemistry continue to grow, making it an exciting field for curious minds and forward-thinking researchers.

Frequently Asked Questions

What is solid state chemistry?

Solid state chemistry is the study of the synthesis, structure, properties, and applications of solid phase materials, particularly crystals and amorphous solids.

How does solid state chemistry differ from traditional chemistry?

Solid state chemistry focuses specifically on the properties and behavior of solid materials,

unlike traditional chemistry which often deals with gases and liquids as well.

What are some common applications of solid state chemistry?

Applications include the development of semiconductors, superconductors, battery materials, catalysts, and magnetic materials.

Why is solid state chemistry important for battery technology?

Solid state chemistry helps in designing and understanding electrode and electrolyte materials that improve battery efficiency, capacity, and safety.

How does solid state chemistry contribute to the development of superconductors?

It enables the synthesis and characterization of materials that exhibit superconductivity, helping to understand their crystal structures and electronic properties.

What role does solid state chemistry play in semiconductor manufacturing?

It assists in creating and manipulating the crystal structure and doping of semiconductor materials to optimize their electrical properties for electronic devices.

Can solid state chemistry help in environmental applications?

Yes, solid state chemistry is used to develop catalysts for pollution control, materials for carbon capture, and sensors for environmental monitoring.

What techniques are commonly used in solid state chemistry for material characterization?

Techniques include X-ray diffraction (XRD), scanning electron microscopy (SEM), solid state NMR, and electron microscopy.

How is solid state chemistry advancing renewable energy technologies?

By developing new materials for solar cells, fuel cells, and energy storage systems, solid state chemistry is improving the efficiency and durability of renewable energy devices.

Additional Resources

Solid State Chemistry and Its Applications: Unlocking the Potential of Materials Science

Solid state chemistry and its applications represent a cornerstone of modern materials science, bridging the gap between fundamental chemical principles and real-world technological innovation. This specialized branch of chemistry focuses on the study of the synthesis, structure, and properties of solid materials, often crystalline in nature, and explores how their atomic arrangements influence functionality. As industries continue to demand advanced materials with tailored properties, solid state chemistry has emerged as an indispensable field, driving progress in electronics, energy storage, catalysis, and beyond.

Understanding Solid State Chemistry

Solid state chemistry delves into the composition and behavior of solids, emphasizing the arrangement of atoms within a material's lattice framework. Unlike molecular chemistry, where discrete molecules predominate, solid state chemistry deals primarily with extended networks of atoms bonded through ionic, covalent, metallic, or van der Waals forces. The field investigates how these bonding types and crystal structures affect physical and chemical properties such as conductivity, magnetism, optical behavior, and thermal stability.

The discipline encompasses a variety of techniques, including X-ray diffraction, electron microscopy, and spectroscopy, to characterize materials at the atomic and nanoscale levels. These methods enable researchers to elucidate crystal structures, identify defects, and monitor phase transitions. Solid state chemistry also integrates computational modeling to predict material properties and design novel compounds with desired functionalities.

Key Features of Solid State Materials

A fundamental aspect of solid state chemistry is understanding how microscopic features translate into macroscopic behavior:

- **Crystal Structure:** The geometric arrangement of atoms, such as cubic, tetragonal, or hexagonal lattices, dictates many physical properties.
- **Defects and Imperfections:** Vacancies, interstitial atoms, and dislocations can dramatically influence electrical conductivity and mechanical strength.
- Phase Behavior: Many solids exhibit polymorphism, where multiple crystal forms exist and interconvert based on temperature or pressure changes.
- **Electronic Properties:** Band structures arising from atomic orbitals determine whether a material behaves as a conductor, semiconductor, or insulator.

Applications Driving Technological Innovation

The practical utility of solid state chemistry lies in its ability to develop new materials that meet the demands of cutting-edge technologies. From everyday electronics to renewable energy systems, the applications are diverse and expanding.

Energy Storage and Conversion

Solid state chemistry has been pivotal in advancing battery technology, particularly lithium-ion and emerging solid-state batteries. By engineering solid electrolytes with high ionic conductivity and chemical stability, researchers aim to improve safety and energy density compared to conventional liquid electrolytes. Materials such as lithium garnets and sulfide-based solids exemplify breakthroughs enabled by solid state synthesis and characterization.

Beyond batteries, solid state catalysts and electrode materials enhance fuel cells and supercapacitors. For instance, perovskite oxides serve as efficient catalysts in oxygen reduction reactions, critical for fuel cell performance. The ability to tailor electronic and ionic transport properties through precise control of crystal chemistry enables optimization of energy conversion devices.

Electronic and Magnetic Materials

Semiconductors, insulators, and superconductors all fall within the purview of solid state chemistry. The electronics industry relies heavily on compounds such as silicon, gallium arsenide, and various oxides engineered for specific band gaps and charge carrier mobilities. Understanding defect chemistry and doping mechanisms allows fine-tuning of conductivity and device efficiency.

Magnetic materials, including ferrites and rare-earth intermetallics, demonstrate how solid state chemistry influences magnetic ordering and anisotropy. These materials underpin applications ranging from data storage to electromagnetic sensors. The interplay between crystal symmetry and magnetic interactions is a rich area of study with ongoing innovation.

Catalysis and Industrial Chemistry

Heterogeneous catalysis often involves solid catalysts whose surfaces facilitate chemical transformations. Solid state chemistry informs the design of catalysts with active sites optimized for selectivity and stability. Zeolites, metal oxides, and mixed-metal frameworks exemplify materials where pore structure and electronic properties are engineered for specific reactions.

Industrial processes such as ammonia synthesis, hydrocarbon cracking, and pollution control depend on catalysts developed through solid state principles. Advances in this area contribute to greener chemical manufacturing and reduced energy consumption.

Pharmaceuticals and Biomaterials

While often associated with inorganic materials, solid state chemistry also plays a role in pharmaceuticals, especially in the development of crystalline drug forms with improved solubility and bioavailability. Polymorphism affects drug stability and efficacy, making solid state analysis critical during formulation.

In biomaterials, solid state chemistry guides the creation of biocompatible ceramics and glass materials used in implants and tissue engineering. Understanding crystallinity and surface chemistry is essential for optimizing interactions with biological environments.

Challenges and Future Directions

Despite significant advances, solid state chemistry faces ongoing challenges. Synthesizing materials with precise atomic arrangements at scale remains complex and often energy-intensive. Predicting properties of novel compounds requires sophisticated computational tools and extensive experimental validation.

Emerging areas such as two-dimensional materials (e.g., graphene and transition metal dichalcogenides) and topological insulators present exciting opportunities but also demand deeper understanding of solid state phenomena at reduced dimensionality. Additionally, integrating sustainable practices into material synthesis aligns with global efforts to minimize environmental impact.

Collaboration across disciplines—combining chemistry, physics, materials science, and engineering—will be crucial in addressing these challenges. The continued development of advanced characterization techniques and machine learning-driven materials discovery promises to accelerate innovation.

Summary

Solid state chemistry and its applications constitute a dynamic field that underpins much of today's technological landscape. By elucidating the relationships between atomic structure and material properties, the discipline enables the design of advanced materials for energy, electronics, catalysis, and healthcare. The interplay of experimental and theoretical approaches continues to push boundaries, promising novel materials with unprecedented capabilities. As global demands evolve, solid state chemistry remains at the forefront of materials innovation, driving progress toward a more efficient and sustainable future.

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solid state chemistry and its applications: Solid State Chemistry and its Applications Anthony R. West, 2022-04-06 SOLID STATE CHEMISTRY AND ITS APPLICATIONS A comprehensive treatment of solid state chemistry complete with supplementary material and full colour illustrations from a leading expert in the field. Solid State Chemistry and its Applications, Second Edition delivers an advanced version of West's classic text in solid state chemistry, expanding on the undergraduate Student Edition to present a comprehensive treatment of solid state chemistry suitable for advanced students and researchers. The book provides the reader with an up-to-date account of essential topics in solid state chemistry and recent developments in this rapidly developing field of inorganic chemistry. Significant updates and new content in this second edition include: A more extensive overview of important families of inorganic solids including spinels, perovskites, pyrochlores, garnets, Ruddlesden-Popper phases and many more New methods to synthesise inorganic solids, including sol-gel methods, combustion synthesis, atomic layer deposition, spray pyrolysis and microwave techniques Advances in electron microscopy, X-ray and electron spectroscopies New developments in electrical properties of materials, including high Tc superconductivity, lithium batteries, solid oxide fuel cells and smart windows Recent developments in optical properties, including fibre optics, solar cells and transparent conducting oxides Advances in magnetic properties including magnetoresistance and multiferroic materials Homogeneous and heterogeneous ceramics, characterization using impedance spectroscopy Thermoelectric materials, MXenes, low dimensional structures, memristors and many other functional materials Expanded coverage of glass, including metallic and fluoride glasses, cement and concrete, geopolymers, refractories and structural ceramics Overview of binary oxides of all the elements, their structures, properties and applications Featuring full color illustrations throughout, readers will also benefit from online supplementary materials including access to CrystalMaker® software and over 100 interactive crystal structure models. Perfect for advanced students seeking a detailed treatment of solid state chemistry, this new edition of Solid State Chemistry and its Applications will also earn a place as a desk reference in the libraries of experienced researchers in chemistry, crystallography, physics, and materials science.

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solid state chemistry and its applications: High Magnetic Field Science and Its Application in the United States National Research Council, Division on Engineering and Physical Sciences, Board on Physics and Astronomy, Committee to Assess the Current Status and Future Direction of High Magnetic Field Science in the United States, 2013-11-25 The Committee to Assess the Current Status and Future Direction of High Magnetic Field Science in the United States was convened by the National Research Council in response to a request by the National Science Foundation. This report answers three questions: (1) What is the current state of high-field magnet

science, engineering, and technology in the United States, and are there any conspicuous needs to be addressed? (2) What are the current science drivers and which scientific opportunities and challenges can be anticipated over the next ten years? (3) What are the principal existing and planned high magnetic field facilities outside of the United States, what roles have U.S. high field magnet development efforts played in developing those facilities, and what potentials exist for further international collaboration in this area? A magnetic field is produced by an electrical current in a metal coil. This current exerts an expansive force on the coil, and a magnetic field is high if it challenges the strength and current-carrying capacity of the materials that create the field. Although lower magnetic fields can be achieved using commercially available magnets, research in the highest achievable fields has been, and will continue to be, most often performed in large research centers that possess the materials and systems know-how for forefront research. Only a few high field centers exist around the world; in the United States, the principal center is the National High Magnetic Field Laboratory (NHMFL). High Magnetic Field Science and Its Application in the United States considers continued support for a centralized high-field facility such as NHFML to be the highest priority. This report contains a recommendation for the funding and siting of several new high field nuclear magnetic resonance magnets at user facilities in different regions of the United States. Continued advancement in high-magnetic field science requires substantial investments in magnets with enhanced capabilities. High Magnetic Field Science and Its Application in the United States contains recommendations for the further development of all-superconducting, hybrid, and higher field pulsed magnets that meet ambitious but achievable goals.

solid state chemistry and its applications: Thermal Decomposition of Ionic Solids A.K. Galwey, M.E. Brown, 1999-02-25 The principal objective of this book is to stimulate interest in research that will extend available theory towards a greater understanding of the steps involved in solid-state decompositions and the properties of solids that control reactivities. Much of the activity in this field has been directed towards increasing the range of reactants for which decomposition kinetic data is available, rather than extending insights into the fundamental chemistry of the reactions being studied. The first part of the book (Chapters 1-6) is concerned with theoretical aspects of the subject. The second part (Chapters 7-17) surveys groups of reactions classified by similarities of chemical composition. The final Chapter (18) reviews the subject by unifying features identified as significant and proposes possible directions for future progress. Studies of thermal reactions of ionic compounds have contributed considerably to the theory of solid-state chemistry. Furthermore, many of these rate processes have substantial technological importance, for example, in the manufacture of cement, the exploitation of ores and in the stability testing of drugs, explosives and oxidizing agents. Despite the prolonged and continuing research effort concerned with these reactions, there is no recent overall review. This book is intended to contribute towards correcting this omission. The essential unity of the subject is recognized by the systematic treatment of reactions, carefully selected to be instructive and representative of the subject as a whole. The authors have contributed more than 200 original research articles to the literature, many during their 25 years of collaboration. Features of this book: • Gives a comprehensive in-depth survey of a rarely-reviewed subject. • Reviews methods used in studies of thermal decompositions of solids. • Discusses patterns of subject development perceived from an extensive literature survey. This book is expected to be of greatest value and interest to scientists concerned with the chemical properties and reactions of solids, including chemists, physicists, pharmacists, material scientists, crystallographers, metallurgists and others. This wide coverage of the literature dealing with thermal reactions of solids will be of value to both academic and industrial researchers by reviewing the current status of the theory of the subject. It could also provide a useful starting point for the exploitation of crystalline materials in practical and industrial applications. The contents will also be relevant to a wide variety of researchers, including, for example, those concerned with the stabilities of polymers and composite materials, the processing of minerals, the shelf-lives of pharmaceuticals, etc.

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2025-01-27 Inorganic Chemistry Fourth Edition provides essential information for students of inorganic chemistry and is updated throughout. The presentation of topics is made with an effort to be clear and concise so that the book is portable and user friendly. The text emphasizes fundamental principles—including molecular structure, acid-base chemistry, coordination chemistry, ligand field theory, and solid state chemistry. It is organized into five major themes (structure, condensed phases, solution chemistry, main group and coordination compounds) with several chapters in each. There is a logical progression from atomic structure to molecular structure to properties of substances based on molecular structures, to behavior of solids, etc. The textbook contains a balance of topics in theoretical and descriptive chemistry. For example, the hard-soft interaction principle is used to explain hydrogen bond strengths, strengths of acids and bases, stability of coordination compounds, etc. Discussion of elements begins with survey chapters focused on the main groups, while later chapters cover the elements in greater detail. Each chapter opens with narrative introductions and includes figures, tables, and end-of-chapter problem sets. This new edition features updates throughout, with an emphasis on bioinorganic chemistry and a new chapter on nanostructures and graphene. More in-text worked-out examples encourage active learning and prepare students for their exams. This text is ideal for advanced undergraduate and graduate-level students enrolled in the Inorganic Chemistry course. This core course serves Chemistry and other science majors. The book may also be suitable for biochemistry, medicinal chemistry, and other professionals who wish to learn more about this subject area. - Physical chemistry is incorporated to show the relevant principles from bonding theory and thermodynamics, while also emphasizing the chemical characteristics of main group elements and coordination chemistry - An extensive revision to the bioinorganic chemistry chapter brings the student up to date on cutting edge research -Discussion of elements begins with survey chapters focused on the main groups, while later chapters cover the elements in greater detail - Each chapter opens with narrative introductions and includes figures, tables, and end-of-chapter problem sets New to this edition - More descriptive language, sentences flow more logically than they do in numerous chemistry books - Additional coverage on topics as photovoltaic compounds, metal oxide catalysts, superconductivity, flame fusion synthesis, splitting water, nanoparticles synthesis and use, high temperature syntheses - Updated end of chapter exercises

solid state chemistry and its applications: Supercapacitors Syam G. Krishnan, Hong Duc Pham, Deepak P. Dubal, 2024-03-20 Supercapacitors: Materials, Design, and Commercialization provides a comprehensive overview of the latest research trends and opportunities in supercapacitors, and particularly in terms of novel materials and electrolytes. The book will address the transformation in supercapacitive technology from double layer capacitance to battery-type capacitance, providing a clear understanding of the conceptual differences between various charge storage processes for supercapacitors, charge storage based on materials and electrolytes, and calculation for capacitance for these charge processes. Detailed chapters discuss recent developments in materials, such as carbons, chalcogenides, MXene and phosphorene, various polymer nanocomposites, and polyoxometalates for supercapacitors. This is followed by in-depth coverage of electrolytes, including the evolution of electrolytes from agueous to water-in-salt electrolytes and their role in improving the energy density of supercapacitors. The final part of the book examines the role of artificial intelligence in the design of supercapacitors, and latest developments in translating novel supercapacitor technologies from laboratory-scale research to a commercialization. This is a valuable resource for advanced students, researchers, and scientists in the fields of energy storage, electrical engineering, materials science, and chemical engineering, as well as engineers and R&D personnel working with supercapacitors or energy storage in an industrial setting. - Brings together the latest developments in supercapacitor materials and electrolytes - Discusses cutting-edge charge storage concepts and methods for supercapacitors -Addresses the role of machine learning and the scale-up from laboratory to commercialization

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areas. It begins with three broad topics: how and why atoms bind together to form solids, lattice vibrations and phonons, and electrons in solids. It then applies this knowledge to interactions, especially those between electrons and phonons, metals, the Fermi surface and alloys, semiconductors, magnetism, superconductivity, dielectrics and ferroelectrics, optical properties, defects, layered materials, quantum Hall effect, mesoscopics, nanophysics and soft condensed matter. Further important topics of the book are the evolution of BEC to BCS phenomena, conducting polymers, graphene, iron pnictide superconductors, light emitting diodes, N-V centers, nanomagnetism, negative index of refraction, optical lattices, phase transitions, phononics, photonics, plasmonics, quantum computing, solar cells, spin Hall effect and spintronics. In this 3rd edition, topics such as topological insulators, quantum computing, Bose-Einstein transitions, highly correlated electron systems and several others have been added. New material on magnetism in solids, as well as a discussion of semiconductors and a changed set of problems with solutions, are also included. The book also discusses "folk theorems" to remind readers of the essence of the physics without mathematics, and includes 90 mini-biographies of prominent solid state physicists of the past and present to put a human face on the subject. An extensive solutions manual rounds out the book.

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It takes into account the many developments that have taken place in the field over the past few decades due to the rapid advances in quantum chemical models and faster computers. This is the perfect complement to Chemical Bonding - Fundamentals and Models by the same editors, who are two of the top scientists working on this topic, each with extensive experience and important connections within the community.

solid state chemistry and its applications: Solids and Surfaces Roald Hoffmann, 2021-01-29 Dieses einzigartige Buch läßt Chemie und Physik im festen Zustand und auf Oberflächen 'zusammentreffen'. In einer lebhaften und anschaulichen Weise bringt es Chemikern die Sprache bei, mit der sie die Elektronenstruktur ausgedehnter Systeme verstehen lernen können. Gleichzeitig zeigt es, wie auch von Seiten der Chemie Modelle über den festen Zustand sowie über Bindungen und Reaktivität von Oberflächen erstellt werden können. Das Buch bedient sich zunächst der Sprache von Kristallorbitalen, Bandstrukturen und Zustandsdichten. Danach stellt es die Werkzeuge bereit, mit denen der Leser weg von den stark delokalisierten Orbitalen des Festkörpers gelangt, darunter der Zerfall von Zustandsdichten und die Population von Kristallorbital-Overlaps. Mit diesen Werkzeugen schafft es der Autor, detaillierte quantenmechanische Berechnungen mit der chemischen Betrachtungsweise mit Grenzorbitalen zu verknüpfen. Die beschriebenen Anwendungen umfassen eine allgemeine Vorstellung der Chemisorption, Bindungsbildung und -zerfall im festen Zustand, Bindungen im Metall, die Elektronenstruktur ausgewählter leitender und supraleitender Verbindungen sowie die für die Deformation ausgedehnter Systeme verantwortlichen Kräfte.

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