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1YRJYK - HUANG CARR

This revision of the introductory textbook of physical chemistry has been designed to broaden its appeal, particularly to students with an interest in biological applications.

The book is a multi-author survey (in 15 chapters) of the current state of knowledge and recent developments in our understanding of oxide surfaces. The author list includes most of the acknowledged world experts in this field. The material covered includes fundamental theory and experimental studies of the geometrical, vibrational and electronic structure of such surfaces, but with a special emphasis on the chemical properties and associated reactivity. The main focus is on metal oxides but coverage extends from 'simple' rock-salt materials such as MgO through to complex transition metal oxides with different valencies.

In flow chemistry reactions are performed in a reactor with the reactants pumped through it. It has the benefit of being easily scaled up and it is straightforward to integrate synthesis, workup and analysis into one system. This volume provides an update on recent advances in the field of flow chemistry, with special emphasis on new, integrated approaches for green and efficient chemistry. This book is a valuable resource for researchers in green chemistry, chemical engineers and Industrial chemists working in the pharmaceutical and fine chemicals industries.

This definitive reference consolidates current knowledge on dihydrogen bonding, emphasizing its role in organizing interactions in different chemical reactions and molecular aggregations. After an overview, it analyzes the differences between dihydrogen bonds, classical hydrogen bonds, and covalent bonds. It describes dihydrogen bonds as intermediates in intramolecular and intermolecular proton transfer reactions. It describes dihydrogen bonding in the solid-state, the gas phase, and in solution. This is the premier reference for physical chemists, biochemists, biophysicists, and chemical engineers.

Providing a general approach to understanding the properties of

molecules and crystals and their origins, the Jahn-Teller effect is a fascinating phenomena in modern physics and chemistry. Its effect inspired one of the most important recent scientific discoveries--the concept of high-temperature superconductivity. This comprehensive volume presents the background of the theory and its key applications in physics and chemistry, as well as more recent achievements.

This book describes the rapidly expanding field of two-dimensional (2D) transition metal carbides and nitrides (MXenes). It covers fundamental knowledge on synthesis, structure, and properties of these new materials, and a description of their processing, scale-up and emerging applications. The ways in which the quickly expanding family of MXenes can outperform other novel nanomaterials in a variety of applications, spanning from energy storage and conversion to electronics; from water science to transportation; and in defense and medical applications, are discussed in detail.

Specific ion effects are important in numerous fields of science and technology. They have been discussed for over 100 years, ever since the pioneering work done by Franz Hofmeister and his group in Prague. Over the last decades, hundreds of examples have been published and periodically explanations have been proposed. However, it is only recently that a profound understanding of the basic effects and their reasons could be achieved. Today, we are not far from a general explanation of specific ion effects. This book summarizes the main new ideas that have come up in the last ten years. In this book, the efforts of theoreticians are substantially supported by the experimental results stemming from new and exciting techniques. Both the new theoretical concepts and the experimental landmarks are collected and critically discussed by eminent scientists and well-known specialists in this field. Beyond the rigorous explanations, guidelines are given to non-specialists in order to help them understand the general rules governing specific ion effects in chemistry, biology, physics and engineering. Sample Chapter(s). Foreword (36 KB). Chapter 1: An Attempt of a General Overview (1,279 KB). Contents: Examples, Ion Properties and Concepts: An Attempt of a General Overview (W Kunz & R Neueder); Phospholipid Aggregates as Model Systems to Understand Ion-Specific Effects: Experiments and Models (E Leontidis); Modelling Specific Ion Effects in Engineering Science (C Held & G Sadowski); Promising Experimental Techniques: Linear and Non-linear Optical Techniques to Probe Ion Profiles at the AirOCoWater Interface (H Motschmann & P Koelsch); X-Ray Studies of Ion Specific Effects (P Viswanath et al.); The Determination of Specific Ion Structure by Neutron Scattering and Computer Simulation (G W Neilson et al.); Specific Ion Effects at the AirOCoWater Interface: Experimental Studies (V S J Craig & C L Henry); Newest Results from Theory and Simulation: Ion Binding to Biomolecules (M Lund et al.); Ion-Specificity: From Solvation Thermodynamics to Molecular Simulations and Back (J Dzubiella et al.); HNC Calculations of Specific Ion Effects (L Belloni & I Chikina); Modifying the PoissonOCoBoltzmann Approach to Model Specific Ion Effects (M BostrAm et al.); Summary and Conclusions: An Attempt of a Summary (W Kunz & G J T Tiddy). Readership: Graduate students and research-

ers in physical chemistry, biological chemistry and chemical engineering; colloidal scientists."

New and Future Developments in Catalysis is a package of books that compile the latest ideas concerning alternate and renewable energy sources and the role that catalysis plays in converting new renewable feedstock into biofuels and biochemicals. Both homogeneous and heterogeneous catalysts and catalytic processes will be discussed in a unified and comprehensive approach. There will be extensive cross-referencing within all volumes. This volume presents a complete picture of all carbon dioxide (CO2) sources, outlines the environmental concerns regarding CO2, and critically reviews all current CO2 activation processes. Furthermore, the volume discusses all future developments and gives a critical economic analysis of the various processes.

Thorough and up-to-date, this book presents recent developments in this exciting research field. To begin with, the text covers the fabrication of chiral nanomaterials via various synthesis methods, including electron beam lithography, ion beam etching, chemical synthesis and biological DNA directed assembly. This is followed by the relevant theory and reaction mechanisms, with a discussion of the characterization of chiral nanomaterials according to the optical properties of metal nanoparticles, semiconductor nanocrystals, and nanoclusters. The whole is rounded off by a summary of applications in the field of catalysis, sensors, and biomedicine. With its comprehensive yet concise coverage of the whole spectrum of research, this is invaluable reading for senior researchers and entrants to the field of nanoscience and materials science.

"This book is about Emerging Trends in Chemical Applications of Lasers"--

Physical Sciences Data, Volume 16: Gaussian Basis Sets for Molecular Calculations provides information pertinent to the Gaussian basis sets, with emphasis on lithium, radon, and important ions. This book discusses the polarization functions prepared for lithium through radon for further improvement of the basis sets. Organized into three chapters, this volume begins with an overview of the basis set for the most stable negative and positive ions. This text then explores the total atomic energies given by the basis sets. Other chapters consider the distinction between diffuse functions and polarization function. This book presents as well the exponents of polarization function. The final chapter deals with the Gaussian basis sets. This book is a valuable resource for chemists, scientists, and research workers.

Real insight from leading experts in the field into the causes of the unique photovoltaic performance of perovskite solar cells, describing the fundamentals of perovskite materials and device architectures. The authors cover materials research and development, device fabrication and engineering methodologies, as well as current knowledge extending beyond perovskite photovoltaics, such as the novel spin physics and multiferroic properties of this family of materials. Aimed at a better and clearer understanding of the latest developments in the hybrid perovskite field, this is a must-have for material scientists, chemists, physicists and engineers entering or already working in this booming field.

Offering the latest informa-

tion in magnetic nanoparticle (MNP) research, this book builds upon the success of the first volume and provides an updated and comprehensive review, from synthesis, characterization, and biofunctionalization to clinical applications of MNPs, including the diagnosis and treatment of cancers. The book captures some of emerging research area which was not available in the first volume. Good Manufacturing Practices and Commercialization of MNPs are also included. This volume, also written by some of the most qualified experts in the field, incorporates new developments in the literature, and continues to bridge the gaps between the different areas in this field.

The developments in the area of ordered nanoporous solids have moved beyond the traditional catalytic and separation uses and given rise to a wide variety of new applications in different branches of chemistry, physics, material science, etc. The activity in this area is due to the outstanding properties of nanoporous materials that have attracted the attention of researchers from different communities. However, recent achievements in a specific field often remain out of the focus of collaborating communities. This work summarizes the latest developments and prospects in the area of ordered porous solids, including synthetic layered materials (clays), microporous zeolite-type materials, ordered mesoporous solids, metal-organic-framework compounds (MOFs), carbon, etc. All aspects, from synthesis via comprehensive characterization to the advanced applications of ordered porous materials, are presented. The chapters are written by leading experts in their respective fields with an emphasis on recent progress and the state of the art. * Summarizes the latest developments in the field of ordered nanoporous solids * Presents state-of-the-art coverage of applications related to porous solids * Incorporates 28 contributions from experts across the disciplines

This book discusses current techniques and instrumentation for cluster chemistry. It addresses both the experimental and theoretical aspects of gas-phase metal cluster reactivities, especially those pertaining to pollution removal, energetic reactions and corrosion and anticorrosion. These metal cluster systems have attracted enormous interest as they display a completely new class of physical, chemical, electronic, magnetic and catalytic properties. As these properties change with size and composition, it can thus be understood how their nature evolves from atoms to bulk solids. The book offers readers a basic understanding of the structural chemistry and reactivity of metal clusters in both gas-phase and wet chemistry. Further, the lessons they learn here regarding metal cluster chemistry will prepare researchers for the study of condensed phase dynamics that pertain to wet chemical synthesis, soft-landing deposition and cluster assembly. A wealth of information in one accessible book. Written by international experts from multidisciplinary fields, this in-depth exploration of oxide ultrathin films covers all aspects of these systems, starting with preparation and characterization, and going on to geometrical and electronic structure, as well as applications in current and future systems and devices. From the Contents: Synthesis and Preparation of Oxide Ultrathin Films Characterization Tools of Oxide Ultrathin Films Ordered Oxide

Nanostructures on Metal Surfaces Unusual Properties of Oxides and Other Insulators in the Ultrathin Limit Silica and High-K Dielectrics Thin Films in Microelectronics Oxide Passive Films and Corrosion Protection Oxide Films as Catalytic Materials and as Models of Real Catalysts Oxide Films in Spintronics Oxide Ultrathin Films in Solid Oxide Fuel Cells Transparent Conducting and Chromogenic Oxide Films as Solar Energy Materials Oxide Ultrathin Films in Sensor Applications Ferroelectricity in Ultrathin Film Capacitors Titania Thin Films in Biocompatible Materials and Medical Implants Oxide Nanowires for New Chemical Sensor Devices

Explains the underlying structure that unites all disciplinesin chemistry Now in its second edition, this book explores organic,organometallic, inorganic, solid state, and materials chemistry,demonstrating how common molecular orbital situations arisethroughout the whole chemical spectrum. The authors explore therelationships that enable readers to grasp the theory thatunderlies and connects traditional fields of study withinchemistry, thereby providing a conceptual framework with which tothink about chemical structure and reactivity problems. Orbital Interactions in Chemistry begins by developingmodels and reviewing molecular orbital theory. Next, the bookexplores orbitals in the organic-main group as well as in solids.Lastly, the book examines orbital interaction patterns that occurin inorganic–organometallic fields as well as clusterchemistry, surface chemistry, and magnetism in solids. This Second Edition has been thoroughly revised andupdated with new discoveries and computational tools since thepublication of the first edition more than twenty-five years ago.Among the new content, readers will find: Two new chapters dedicated to surface science and magneticproperties Additional examples of quantum calculations, focusing oninorganic and organometallic chemistry Expanded treatment of group theory New results from photoelectron spectroscopy Each section ends with a set of problems, enabling readers totest their grasp of new concepts as they progress through the text.-Solutions are available on the book's ftp site. Orbital Interactions in Chemistry is written for bothresearchers and students in organic, inorganic, solid state,-materials, and computational chemistry. All readers will discoverthe underlying structure that unites all disciplines inchemistry.

Nanocatalysis, a subdiscipline of nanoscience, seeks to control chemical reactions by changing the size, dimensionality, chemical composition, and morphology of the reaction center and by changing the kinetics using nanopatterning of the reaction center. This book offers a detailed pedagogical and methodological overview of the field. Readers discover many examples of current research, helping them explore new and emerging applications.

Chemistry: A Guided Approach 6th Edition follows the underlying principles developed by years of research on how readers learn and draws on testing by those using the POGIL methodology. This text follows inquiry based learning and correspondingly emphasizes the underlying concepts and the reasoning behind the concepts. This text offers an approach that follows modern cognitive learning principles by having readers learn how to create knowledge based on experimental data and how

to test that knowledge.
"This book is about Free Energy Methods in Drug Discovery: Current State and Future Directions"--

A guide to taking the Advanced Placement Chemistry exam, featuring three full-length practice tests, one diagnostic test, in-depth subject reviews, and a guide to AP credit and placement. Includes CD-ROM with information on financing a college degree.

This book develops the subject from the basic principles of quantum mechanics. The emphasis is on a single statement of the ideas underlying the various approximations that have to be used and care is taken to separate sound arguments from conjecture. This book is written for the student of theoretical physics who wants to work in the field of solids and for the experimenter with a knowledge of quantum theory who is not content to take other people's arguments for granted. The treatment covers the electron theory of metals as well as the dynamics of crystals, including the author's work on the thermal conductivity of crystals which has been previously published in English.

The Chemistry of the Actinide and Transactinide Elements is a contemporary and definitive compilation of chemical properties of all of the actinide elements, especially of the technologically important elements uranium and plutonium, as well as the transactinide elements. In addition to the comprehensive treatment of the chemical properties of each element, ion, and compound from atomic number 89 (actinium) through to 109 (meitnerium), this multi-volume work has specialized and definitive chapters on electronic theory, optical and laser fluorescence spectroscopy, X-ray absorption spectroscopy, organoactinide chemistry, thermodynamics, magnetic properties, the metals, coordination chemistry, separations, and trace analysis. Several chapters deal with environmental science, safe handling, and biological interactions of the actinide elements. The Editors invited teams of authors, who are active practitioners and recognized experts in their specialty, to write each chapter and have endeavoured to provide a balanced and insightful treatment of these fascinating elements at the frontier of the periodic table. Because the field has expanded with new spectroscopic techniques and environmental focus, the work encompasses five volumes, each of which groups chapters on related topics. All chapters represent the current state of research in the chemistry of these elements and related fields.

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.

Because of the importance of the hydrogen bond, there have been scores of insights gained about its fundamental nature by quantum chemical computations over the years. Such methods can probe subtle characteristics of the electronic structure and examine regions of the potential energy surface that are simply not accessible by experimental means. The maturation of the techniques, codes, and computer hardware have permitted calculations of unprecedented reliability and rivaling the accuracy of experimental data. This book strives first toward an appreciation of the power of quantum chemistry to analyze the deepest roots of the hydrogen bond phenomenon. It offers a systematic and understandable account of decades of such calculations, focusing on the most important findings. This book provides readers with the tools to understand the original literature, and to perhaps carry out some calculations of their very own on systems of interest.

Photochemical reactions and the underlying photophysical principles play key roles in the rational design of efficient systems for energy conversion and storage. This volume on interfaces contains fundamental theory, computational models, and applications for real materials. Edited by experts with a deep knowledge of the community, the volume will be useful to computational chemists, materials scientists, physical chemists, and especially those working in energy and nanomaterials.

This book reflects the current status of theoretical and experimental research of graphene based nanostructures, in particular quantum dots, at a level accessible to young researchers, graduate students, experimentalists and theorists. It presents the current state of research of graphene quantum dots, a single or few monolayer thick islands of graphene. It introduces the reader to the electronic and optical properties of graphite, intercalated graphite and graphene, including Dirac fermions, Berry's phase associated with sublattices and valley degeneracy, covers single particle properties of graphene quantum dots, electron-electron interaction, magnetic properties and optical properties of gated graphene nanostructures. The electronic, optical and magnetic properties of the graphene quantum dots as a function of size, shape, type of edge and carrier density are considered. Special attention is paid to the understanding of edges and the emergence of edge states for zigzag edges. Atomistic tight binding and effective mass approaches to single particle calculations are performed. Furthermore, the theoretical and numerical treatment of electron-electron interactions at the mean-field, HF, DFT and configuration-interaction level is described in detail.

Spin Dynamics: Basics of Nuclear Magnetic Resonance, Second Edition is a comprehensive and modern introduction which focuses on those essential principles and concepts needed for a thorough understanding of the subject, rather than the practical aspects. The quantum theory of nuclear magnets is presented within a strong physical framework, supported by figures. The book assumes only a basic knowledge of complex numbers and matrices, and provides the reader with numerous worked examples and exercises to encour-

age understanding. With the explicit aim of carefully developing the subject from the beginning, the text starts with coverage of quarks and nucleons and progresses through to a detailed explanation of several important NMR experiments, including NMR imaging, COSY, NOESY and TROSY. Completely revised and updated, the Second Edition features new material on the properties and distributions of isotopes, chemical shift anisotropy and quadrupolar interactions, Pake patterns, spin echoes, slice selection in NMR imaging, and a complete new chapter on the NMR spectroscopy of quadrupolar nuclei. New appendices have been included on Euler angles, and coherence selection by field gradients. As in the first edition, all material is heavily supported by graphics, much of which is new to this edition. Written for undergraduates and postgraduate students taking a first course in NMR spectroscopy and for those needing an up-to-date account of the subject, this multi-disciplinary book will appeal to chemical, physical, material, life, medical, earth and environmental scientists. The detailed physical insights will also make the book of interest for experienced spectroscopists and NMR researchers. • An accessible and carefully written introduction, designed to help students to fully understand this complex and dynamic subject • Takes a multi--disciplinary approach, focusing on basic principles and concepts rather than the more practical aspects • Presents a strong pedagogical approach throughout, with emphasis placed on individual spins to aid understanding • Includes numerous worked examples, problems, further reading and additional notes Praise from the reviews of the First Edition: "This is an excellent book... that many teachers of NMR spectroscopy will cherish... It deserves to be a 'classic' among NMR spectroscopy texts." NMR IN BIOMEDICINE "I strongly recommend this book to everyone...it is probably the best modern comprehensive description of the subject." ANGEWANDTE CHEMIE, INTERNATIONAL EDITION

The book presents the fundamental aspects of surface segregation theory. The material is presented in a self-contained manner and mathematical procedures are worked through in some cases in order to provide the reader with the necessary opportunity to realize the restrictions under which the expressions are valid.

Nanoclusters' potential applications include microelectronics, magnetic storage, optical data storage, spintronics devices, telecommunications, sensors, transducers, biological markers, switches, electroluminescent displays, chemical reactors, and catalysts, among others; nanocrystalline materials w

This book gives a theoretical description of linear and nonlinear optical responses of matter with special emphasis on the microscopic and 'nonlocal' nature of resonant response. It will have a tremendous influence on modern device techniques, as it deals with frontier research in response theory.

This first volume in the series brings together the latest developments in solid surface photochemistry, providing insights into the most up to date research activities on light-initiated chemical reactions. The book offers a comprehensive study of the photochemical and photophysical properties of molecules on various surfaces like zeolites, metals and metal oxides.

Chapter 1 discusses the nature of the photochemical and photophysical reactions occurring on solid surfaces. Subsequent chapters deal with a description of the dynamical aspects of surface photochemistry, a study of the specific nature of photochemistry of molecules included within zeolite cavities and a comprehensive study of the reactivities of photo-generated electron--hole pair states involved in photo-induced and photocatalytic reactions. The book also investigates many possible and actual key applications of solid surface photochemistry, such as molecular photo-devices, photo-chemical vapour deposition of thin layered semiconductors, sensitive optical media and control of photochemical reaction paths as well as efficient photocatalytic reaction processes which will be indispensable for ecologically clean and safe chemical systems. Surface Photochemistry will be of interest to researchers in surface science and also to graduate students interested in catalysis or photo-chemistry. It will be valuable as a reference book for academics in many aspects of materials science.

Reducing the size of a coherently grown semiconductor cluster in all three directions of space to a value below the de Broglie wavelength of a charge carrier leads to complete quantization of the energy levels, density of states, etc. Such “quantum dots” are more similar to giant atoms in a dielectric cage than to classical solids or semiconductors showing a dispersion of energy as a function of wavevector. Their electronic and optical properties depend strongly on their size and shape, i.e. on their geometry. By designing the geometry by controlling the growth of QDs, absolutely novel possibilities for material design leading to novel devices are opened. This multiauthor book written by world-wide recognized leaders of their particular fields and edited by the recipient of the Max-Born Award and Medal 2006 Professor Dieter Bimberg reports on the state of the art of the growing of quantum dots, the theory of self-organised growth, the theory of electronic and excitonic states, optical properties and transport in a variety of materials. It covers the subject from the early work beginning of the 1990s up to 2006. The topics addressed in the book are the focus of research in all leading semiconductor and optoelectronic device laboratories of the world.

The authors of this book are pioneers of the passive, integrative sampling approach and developers of globally applied semipermeable membrane devices (SPMDs). The book will boost understanding of how passive samplers such as SPMD function by examining basic exchange processes that mediate the concentration of SVOCs in a sampling matrix. The book delineates fundamental theory and modeling techniques, while providing a practical guide for its proper application.

A comprehensive volume on interfacial catalysis, this book includes contributions from an international group of specialists in chemistry, environmental science, informatics, physiology, nuclear energy, and physics. The editor has organized the material into the main topics of fundamental characteristics, phase transfer catalysis, reversed micelles, biological aspects, and interfacial photocatalysis. Individual topics include self--organized microheterogeneous structures, nanochemistry, interfacial catalysis in metal complexation, the role of water

molecules in ion transfer at the oil/water interface, and ultrathin films in enhanced oil recovery.