Chemistry And Chemical Reactivity Hybrid Edition With Printed Access Card 24 Months To Owl With Cengage Youbook Cengage Learnings New Hybrid Editions

A modern, comprehensive text and reference describing intermolecular forces, this book begins with coverage of the concepts and methods for simpler systems, then moves on to more advanced subjects for complex systems – emphasizing concepts and methods used in calculations with realistic models and compared with empirical data. Contains applications to many physical systems and worked examples Proceeds from introductory material to advanced modern treatments Has relevance for new materials, biological phenomena, and energy and fuels production
Reflecting Cengage Learning's commitment to offering flexible teaching solutions and value for students and instructors, this new hybrid version features the instructional presentation found in the printed text while delivering all the end-of chapter exercises online in OWLv2, the leading online learning system for chemistry. The result--a briefer printed text that engages learners online! Improve your grades and understanding of concepts with this value-packed Hybrid Edition. An access code to OWLv2 with MindTap Reader is included with the text, providing powerful online resources that include tutorials, simulations, randomized homework questions, videos, a complete interactive electronic version of the textbook, and more! Succeed in chemistry with the clear explanations, problem-solving strategies, and dynamic study tools of CHEMISTRY & CHEMICAL REACTIVITY, 9th edition. Combining thorough instruction with the powerful multimedia tools you need to develop a deeper understanding of general chemistry concepts, the text emphasizes the visual nature of chemistry, illustrating the close interrelationship of the macroscopic, symbolic, and particulate levels of chemistry. The art program illustrates each of these levels in engaging detail--and is fully integrated with key media components.
This book explains key concepts in theoretical chemistry and explores practical applications in structural chemistry. For experimentalists, it highlights concepts that explain the underlying mechanisms of observed phenomena, and at the same time provides theoreticians with explanations of the principles and techniques that are important in property design. Themes covered include conceptual and applied wave functions and density functional theory (DFT) methods, electronegativity and hard and soft (Lewis) acid and base (HSAB) concepts, hybridization and aromaticity, molecular magnetism, spin transition and thermochromism. Offering insights into designing new properties in advanced functional materials, it is a valuable resource for undergraduates of physical chemistry, cluster chemistry and structure/reactivity courses as well as graduates and researchers in the fields of physical chemistry, chemical modeling and functional materials.
Papers presenting the theory of chemical reactions and the comparison with experiment.
Author Jennifer MacKay focuses on the invention of electric cars, exploring how it was developed, how it works, its impact on society, and possible future uses.
Chemistry and Chemical Reactivity - HybridBrooks/Cole Publishing Company
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
The book "Chemical Reactions in Inorganic Chemistry" describes an overview of chemical reagents used in inorganic chemical reactions for the synthesis of different compounds including coordination, transition metal, organometallic, cluster, bioinorganic, and solid-state compounds. This book will be helpful for the graduate students, teachers, and researchers, and chemistry professionals who are interested to fortify and expand their knowledge about sol-gel preparation and application, porphyrin and phthalocyanine, carbon nanotube nanohybrids, triple bond between arsenic and group 13 elements, and N-heterocyclic carbene and its heavier analogues. It comprises a total of five chapters from multiple contributors around the world including China, India, and Taiwan.
Designed to supplement existing organic textbooks, Hybrid Retrosynthesis presents a relatively simple approach to solving synthesis problems, using a small library of basic reactions along with the computer searching capabilities of Reaxys and SciFinder. This clear, concise guide reviews the essential skills needed for organic synthesis and retrosynthesis, expanding reader knowledge of the foundational principles of these techniques, whilst supporting their use via practical methodologies. Perfect for both graduate and post-graduate students, Hybrid Retrosynthesis provides new applied skills and tools to help during their organic synthesis courses and future careers, whilst simultaneously acting as useful resource for those setting tutorial and group problems, and as a helpful go-to guide for organic chemists involved in either industry or academia. Ideal revision and hands on learning guide for organic synthesis Clearly explains the principles and practice of retrosynthesis, which is often not covered in other books Encourages readers to practice their synthetic knowledge supported by real life examples
A quantitative description of the action of enzymes and other biological systems is both a challenge and a fundamental requirement for further progress in our und- standing of biochemical processes. This can help in practical design of new drugs and in the development of artificial enzymes as well as in fundamental understanding of the factors that control the

activity of biological systems. Structural and biochemical st- ies have yielded major insights about the action of biological molecules and the mechanism of enzymatic reactions. However it is not entirely clear how to use this - portant information in a consistent and quantitative analysis of the factors that are - sponsible for rate acceleration in enzyme active sites. The problem is associated with the fact that reaction rates are determined by energetics (i. e. activation energies) and the available experimental methods by themselves cannot provide a correlation - tween structure and energy. Even mutations of specific active site residues, which are extremely useful, cannot tell us about the totality of the interaction between the active site and the substrate. In fact, short of inventing experiments that allow one to measure the forces in enzyme active sites it is hard to see how can one use a direct experimental approach to unambiguously correlate the structure and function of enzymes. In fact, in view of the complexity of biological systems it seems that only computers can handle the task of providing a quantitative structure-function correlation.

The QM/MM method, short for quantum mechanical/molecular mechanical, is a highly versatile approach for the study of chemical phenomena, combining the accuracy of quantum chemistry to describe the region of interest with the efficiency of molecular mechanical potentials to represent the remaining part of the system. Originally conceived in the 1970s by the influential work of the the Nobel laureates Martin Karplus, Michael Levitt and Arieh Warshel, QM/MM techniques have evolved into one of the most accurate and general approaches to investigate the properties of chemical systems via computational methods. Whereas the first applications have been focused on studies of organic and biomolecular systems, a large variety of QM/MM implementations have been developed over the last decades, extending the range of applicability to address research questions relevant for both solution and solid-state chemistry as well. Despite approaching their 50th anniversary in 2022, the formulation of improved QM/MM methods is still an active field of research, with the aim to (i) extend the applicability to address an even broader range of research questions in chemistry and related disciplines, and (ii) further push the accuracy achieved in the QM/MM description beyond that of established formulations. While being a highly successful approach on its own, the combination of the QM/MM strategy with other established theoretical techniques greatly extends the capabilities of the computational approaches. For instance the integration of a suitable QM/MM technique into the highly successful Monte-Carlo and molecular dynamics simulation protocols enables the description of the chemical systems on the basis of an ensemble that is in part constructed on a quantum-mechanical basis. This eBook presents the contributions of a recent Research Topic published in Frontiers in Chemistry, that highlight novel approaches as well as advanced applications of QM/MM method to a broad variety of targets. In total 2 review articles and 10 original research contributions from 48 authors are presented, covering 12 different countries on four continents. The range of research questions addressed by the individual contributions provide a lucid overview on the versatility of the QM/MM method, and demonstrate the general applicability and accuracy that can be achieved for different problems in chemical sciences. Together with the development of improved algorithms to enhance the capabilities of quantum chemical methods and the continuous advancement in the capacities of computational resources, it can be expected that the impact of QM/MM methods in chemical sciences will be further increased already in the near future.

This book is a collection of selected papers on the Frontier Orbital Theory by Nobel prizewinner Kenichi Fukui (Chemistry 1981), with introductory notes. It provides the basic concept and formulation of the theory, and the physical and chemical significance of the frontier orbital interactions in chemistry, together with many practical applications. The formulation of the Intrinsic Reaction Coordinate and applications to some simple systems are also presented. The aim of this volume is to show by what forces chemical reactions are driven and to demonstrate how the regio- and stereo-selectivities are determined in chemical reactions. Students and senior investigators will gain insight into the nature of chemical reactions and find out how quantum chemical calculations are connected with chemical intuition.

A unique selection of papers on the most recent progress in the modelling of biological molecules containing metal ions. New approaches and techniques in this field are allowing researchers to discuss structures, electronic properties and reaction mechanisms of metalloproteins on the basis of computational studies. The book discusses different approaches in the development of new force fields and their application to the computation of the structures, electronic properties and dynamics of bioinorganic compounds as well as quantum mechanical and integrated QM/MM methods for understanding the function of metalloenzymes and the calculation of electrostatic interactions.

This book covers the theory and applications of continuum solvation models. The main focus is on the quantum-mechanical version of these models, but classical approaches and combined or hybrid techniques are also discussed. Devoted to solvation models in which reviews of the theory, the computational implementation Solvation continuum models are treated using the different points of view from experts belonging to different research fields Can be read at two levels: one, more introductive, and the other, more detailed (and more technical), on specific physical and numerical aspects involved in each issue and/or application Possible limitations or incompleteness of models is pointed out with, if possible, indications of future developments Four-colour representation of the computational modeling throughout.

Explore the theory and applications of superatomic clusters and cluster assembled materials Superatoms: Principles, Synthesis and Applications delivers an insightful and exciting exploration of an emerging subfield in cluster science, superatomic clusters and cluster assembled materials. The book presents discussions of the fundamentals of superatom chemistry and their application in catalysis, energy, materials science, and biomedical sciences. Readers will discover the foundational significance of superatoms in science and technology and learn how they can serve as the building blocks of tailored materials, promising to usher in a new era in materials science. The book covers topics as varied as the thermal and thermoelectric properties of cluster-based materials and clusters for CO2 activation and conversion, before concluding with an incisive discussion of trends and directions likely to dominate the subject of superatoms in the coming years. Readers will also benefit from the inclusion of: A thorough introduction to the rational design of superatoms using

electron-counting rules Explorations of superhalogens, endohedrally doped superatoms and assemblies, and magnetic superatoms A practical discussion of atomically precise synthesis of chemically modified superatoms A concise treatment of superatoms as the building blocks of 2D materials, as well as superatom-based ferroelectrics and cluster-based materials for energy harvesting and storage Perfect for academic researchers and industrial scientists working in cluster science, energy materials, thermoelectrics, 2D materials, and CO2 conversion, Superatoms: Principles, Synthesis and Applications will also earn a place in the libraries of interested professionals in chemistry, physics, materials science, and nanoscience.

This comprehensive three-volume handbook brings together a review of the current state together with the latest developments in sol-gel technology to put forward new ideas. The first volume, dedicated to synthesis and shaping, gives an in-depth overview of the wet-chemical processes that constitute the core of the sol-gel method and presents the various pathways for the successful synthesis of inorganic and hybrid organic-inorganic materials, bio- and bio-inspired materials, powders, particles and fibers as well as sol-gel derived thin films, coatings and surfaces. The second volume deals with the mechanical, optical, electrical and magnetic properties of sol-gel derived materials and the methods for their characterization such as diffraction methods and nuclear magnetic resonance, infrared and Raman spectroscopies. The third volume concentrates on the various applications in the fields of membrane science, catalysis, energy research, biomaterials science, biomedicine, photonics and electronics.

The combination of supramolecular chemistry, inorganic solids, and nanotechnology has already led to significant advances in many areas such as sensing, controlled motion, and delivery. By making possible an unprecedented tunability of the properties of nanomaterials, these techniques open up whole new areas of application for future supramolecular concepts. The Supramolecular Chemistry of Organic–Inorganic Hybrid Materials gathers current knowledge on the subject and provides an overview of the present state and upcoming challenges in this rapidly growing, highly cross- or interdisciplinary research field. The book details how these designed materials can improve existing materials or generate novel functional features such as chemical amplification, cooperative binding and signal enhancement that are difficult or not at all achievable by classical organic supramolecular chemistry. It also discusses issues related to nanofabrication or nanotechnology such as the directed and controlled assembly or disassembly, biomimetic functions and strategies, and the gating and switching of surface functions or morphology.

Over the past several decades there have been major advances in our ability to computationally evaluate the electronic structure of inorganic molecules, particularly transition metal systems. This advancement is due to the Moore’s Law increase in computing power as well as the impact of density functional theory (DFT) and its implementation in commercial and freeware programs for quantum chemical calculations. Improved pure and hybrid density functionals are allowing DFT calculations with accuracy comparable to high-level Hartree-Fock treatments, and the results of these calculations can now be evaluated by experiment. When calculations are correlated to, and supported by, experimental data they can provide fundamental insight into electronic structure and its contributions to physical properties and chemical reactivity. This interplay continues to expand and contributes to both improved value of experimental results and improved accuracy of computational predictions. The purpose of this EIC Book is to provide state-of-the-art presentations of quantum mechanical and related methods and their applications, written by many of the leaders in the field. Part 1 of this volume focuses on methods, their background and implementation, and their use in describing bonding properties, energies, transition states and spectroscopic features. Part 2 focuses on applications in bioinorganic chemistry and Part 3 discusses inorganic chemistry, where electronic structure calculations have already had a major impact. This addition to the EIC Book series is of significant value to both experimentalists and theoreticians, and we anticipate that it will stimulate both further development of the methodology and its applications in the many interdisciplinary fields that comprise modern inorganic and bioinorganic chemistry. This volume is also available as part of Encyclopedia of Inorganic Chemistry, 5 Volume Set. This set combines all volumes published as EIC Books from 2007 to 2010, representing areas of key developments in the field of inorganic chemistry published in the Encyclopedia of Inorganic Chemistry. Find out more.

Provides timely, comprehensive coverage of in vivo chemical reactions within live animals This handbook summarizes the interdisciplinary expertise of both chemists and biologists performing in vivo chemical reactions within live animals. By comparing and contrasting currently available chemical and biological techniques, it serves not just as a collection of the pioneering work done in animal-based studies, but also as a technical guide to help readers decide which tools are suitable and best for their experimental needs. The Handbook of In Vivo Chemistry in Mice: From Lab to Living System introduces readers to general information about live animal experiments and detection methods commonly used for these animal models. It focuses on chemistry-based techniques to develop selective in vivo targeting methodologies, as well as strategies for in vivo chemistry and drug release. Topics include: currently available mouse models; biocompatible fluorophores; radionuclides for radiodiagnosis/radiotherapy; live animal imaging techniques such as positron emission tomography (PET) imaging; magnetic resonance imaging (MRI); ultrasound imaging; hybrid imaging; biocompatible chemical reactions; ligand-directed nucleophilic substitution chemistry; biorthogonal prodrug release strategies; and various selective targeting strategies for live animals. -Completely covers current techniques of in vivo chemistry performed in live animals -Describes general information about commonly used live animal experiments and detection methods -Focuses on chemistry-based techniques to develop selective in vivo targeting methodologies, as well as strategies for in vivo chemistry and drug release -Places emphasis on material properties required for the development of appropriate compounds to be used for imaging and therapeutic purposes in preclinical applications Handbook of In Vivo Chemistry in Mice: From Lab to Living System will be of great interest to pharmaceutical chemists, life scientists, and organic chemists. It will also appeal to those working in the pharmaceutical and biotechnology industries.

Polymeric and hybrid nanoparticles have received increased scientific interest in terms of basic research as well as commercial applications, promising a variety of uses for nanostructures in fields including bionanotechnology and medicine. Condensing the relevant research into a comprehensive reference, Polymer and Polymer-Hybrid Nanoparticles: From Synthesis to Biomedical Applications covers an array of topics from synthetic procedures and macromolecular design to possible biomedical applications of nanoparticles and materials based on original and unique polymers. The book presents a well-rounded picture of objects ranging from simple polymeric micelles to complex hybrid polymer-based nanostructures, detailing synthetic procedures, techniques for characterization and analysis, properties, and behavior in selective solvents and dispersions. Each chapter contains background and introductory information, summarizing generalities on the nanosystems being discussed. The chapters also describe representative works of experts and provide in-depth, focused discussions. The authors present current knowledge on the following topics: Designed synthesis of functional polymers Construction of block copolymer micellar and nonmicellar self-assembled structures Construction of organic–organic hybrid nanosized particles Construction of organic–inorganic hybrid nanoparticles and nanoassemblies The final chapter addresses biological applications of polymeric nanoparticles, including delivery of low-molecular-weight drugs, macromolecular drugs, imaging and diagnostics, and photodynamic therapy. Summarizing important developments in the field, the authors condense relevant research into a comprehensive resource.

Succeed in chemistry using this paperback edition of CHEMISTRY & CHEMICAL REACTIVITY, Hybrid with OWL, Eighth Edition, which includes access to OWL Online Web Learning and its built-in interactive eBook. Packed with clear explanations, easy-to-follow problem-solving strategies, and dynamic study tools, the book combines thorough instruction with the powerful multimedia tools you need to develop a deeper understanding of general chemistry concepts. With OWL, you can learn at your own pace to ensure you've mastered each concept before you move on. The authors emphasize the visual nature of chemistry, illustrating the close interrelationship of the macroscopic, symbolic, and particulate levels of chemistry. The book's built-in access to the OWL online learning system helps you maximize your study time and improve your success in the course, while the interactive and customizable Cengage YouBook (interactive eBook) enhances your understanding through videoso and animations and gives you the ability to highlight, add notes, and more--including to option to download GO CHEMISTRY mini video lectures on to the key topics in the text for quick, on-the-go review on your iTunes, video iPods/iPhones, other personal video players, and QuickTime.

Over the last three decades the process industries have grown very rapidly, with corresponding increases in the quantities of hazardous materials in process, storage or transport. Plants have become larger and are often situated in or close to densely populated areas. Increased hazard of loss of life or property is continually highlighted with incidents such as Flixborough, Bhopal, Chernobyl, Three Mile Island, the Phillips 66 incident, and Piper Alpha to name but a few. The field of Loss Prevention is, and continues to, be of supreme importance to countless companies, municipalities and governments around the world, because of the trend for processing plants to become larger and often be situated in or close to densely populated areas, thus increasing the hazard of loss of life or property. This book is a detailed guidebook to defending against these, and many other, hazards. It could without exaggeration be referred to as the "bible" for the process industries. This is THE standard reference work for chemical and process engineering safety professionals. For years, it has been the most complete collection of information on the theory, practice, design elements, equipment, regulations and laws covering the field of process safety. An entire library of alternative books (and cross-referencing systems) would be needed to replace or improve upon it, but everything of importance to safety professionals, engineers and managers can be found in this all-encompassing reference instead. Frank Lees' world renowned work has been fully revised and expanded by a team of leading chemical and process engineers working under the guidance of one of the world’s chief experts in this field. Sam Mannan is professor of chemical engineering at Texas A&M University, and heads the Mary Kay O’Connor Process Safety Center at Texas A&M. He received his MS and Ph.D. in chemical engineering from the University of Oklahoma, and joined the chemical engineering department at Texas A&M University as a professor in 1997. He has over 20 years of experience as an engineer, working both in industry and academia. New detail is added to chapters on fire safety, engineering, explosion hazards, analysis and suppression, and new appendices feature more recent disasters. The many thousands of references have been updated along with standards and codes of practice issued by authorities in the US, UK/Europe and internationally. In addition to all this, more regulatory relevance and case studies have been included in this edition. Written in a clear and concise style, Loss Prevention in the Process Industries covers traditional areas of personal safety as well as the more technological aspects and thus provides balanced and in-depth coverage of the whole field of safety and loss prevention. * A must-have standard reference for chemical and process engineering safety professionals * The most complete collection of information on the theory, practice, design elements, equipment and laws that pertain to process safety * Only single work to provide everything; principles, practice, codes, standards, data and references needed by those practicing in the field

This volume collects research findings presented at the 8th Edition of the Electronic Structure: Principles and Applications (ESPA-2012) International Conference, held in Barcelona, Spain on June 26-29, 2012. The contributions cover research work on methods and fundamentals of theoretical chemistry, chemical reactivity, bimolecular modeling, and materials science. Originally published in the journal Theoretical Chemistry Accounts, these outstanding papers are now available in a hardcover print format, as well as a special electronic edition. This volume provides valuable content for all researchers in theoretical chemistry, and will especially benefit those research groups and libraries with limited access to the journal.

With contributions by numerous experts

There is much interest in using biological structures for the fabrication of new functional materials. Recent developments in the particle character and behaviour of proteins and viral particles have had a major impact on the development of novel nanoparticle systems with new functions and possibilities. Bio-Synthetic Hybrid Materials and Bionanoparticles approaches the subject by covering the basics of disciplines involved as well as recent advances in new materials. The first section of the book focusses on the design and synthesis of different bionanoparticles and hybrid structures including the use of genetic modification as well as by organic synthesis. The second section of the book looks at the self-assembling behaviour of bionanoparticles to form new materials. The final section looks at bionanoparticle-based functional systems and materials including chapters on biomedical applications and electronic systems and devices. Edited by leading scientists in bionanoparticles, the book is a collaboration between scientists with different backgrounds and perspectives which will initiate the next generation of bio-based structures, materials and devices.

An insightful analysis of confined chemical systems for theoretical and experimental scientists Chemical Reactivity in Confined Systems: Theory and Applications presents a theoretical basis for the molecular phenomena observed in confined spaces. The book highlights state-of-

the-art theoretical and computational approaches, with a focus on obtaining physically relevant clarification of the subject to enable the reader to build an appreciation of underlying chemical principles. The book includes real-world examples of confined systems that highlight how the reactivity of atoms and molecules change upon encapsulation. Chapters include discussions on recent developments related to several host-guest systems, including cucurbit[n]uril, ExBox+4, clathrate hydrates, octa acid cavitand, metal organic frameworks (MOFs), covalent organic frameworks (COFs), zeolites, fullerenes, and carbon nanotubes. Readers will learn how to carry out new calculations to understand the physicochemical behavior of confined quantum systems. Topics covered include: A thorough introduction to global reactivity descriptors, including electronegativity, hardness, and electrophilicity An exploration of the Fukui function, as well as dual descriptors, higher order derivatives, and reactivity through information theory A practical discussion of spin dependent reactivity and temperature dependent reactivity Concise treatments of population analysis, reaction force, electron localization functions, and the solvent effect on reactivity Perfect for academic researchers and graduate students in theoretical and computational chemistry and confined chemical systems, Chemical Reactivity in Confined Systems: Theory and Applications will also earn a place in the libraries of professionals working in the areas of catalysis, supramolecular chemistry, and porous materials.

Advanced Topics in Theoretical Chemical Physics is a collection of 20 selected papers from the scientific presentations of the Fourth Congress of the International Society for Theoretical Chemical Physics (ISTCP) held at Marly-le-Roi, France, in July 2002. Advanced Topics in Theoretical Chemical Physics encompasses a broad spectrum in which scientists place special emphasis on theoretical methods in chemistry and physics. The chapters in the book are divided into five sections: I: Advances Chemical Thermodynamics II: Electronic Structure of Molecular Systems III: Molecular Interaction and Dynamics IV: Condensed Matter V: Playing with Numbers This book is an invaluable resource for all academics and researchers interested in theoretical, quantum or statistical, chemical physics or physical chemistry. It presents a selection of some of the most advanced methods, results and insights in this exciting area.

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To accomplish your course goals, use this study guide to enhance your understanding of the text content and to be better prepared for quizzes and tests. This convenient manual helps you assimilate and master the information encountered in the text through the use of practice exercises and applications, comprehensive review tools, and additional helpful resources.

Essentials of Organic Chemistry is an accessible introduction tothe subject for students of Pharmacy, Medicinal Chemistry andBiological Chemistry. Designed to provide a thorough grounding infundamental chemical principles, the book focuses on key elementsof organic chemistry and carefully chosen material is illustratedwith the extensive use of pharmaceutical and biochemicalexamples. In order to establish links and similarities the book placesprominence on principles and deductive reasoning withcross-referencing. This informal text also places the main emphasison understanding and predicting reactivity rather than syntheticmethodology as well as utilising a mechanism based layout andfeaturing annotated schemes to reduce the need for textualexplanations. * tailored specifically to the needs of students of PharmacyMedical Chemistry and Biological Chemistry * numerous pharmaceutical and biochemical examples * mechanism based layout * focus on principles and deductive reasoning This will be an invaluable reference for students of PharmacyMedicinal and Biological Chemistry.

This book is a contribution to the fast and broad Density Functional Theory (DFT) applications of the last few years. Since 2000, the DFT has grown exponentially in several computational areas because of its versatility and reliability to calculate energy from electronic density. The fast DFT’s calculations show how scientists develop more codes focused to simulate molecular and material properties reaching better conclusions than with previous theories. More powerful computers and lower computational costs have certainly assisted the increased growth of interest in this theory. Each chapter presents a specific subject contributing to a vision of the great potential of the quantum/DFT simulations in high pressure, chemical reactivity, ionic liquid, chemoinformatic, molecular docking, and non-equilibrium state.

Succeed in chemistry with the clear explanations, problem-solving strategies, and dynamic study tools of CHEMISTRY & CHEMICAL REACTIVITY, 9e. Combining thorough instruction with the powerful multimedia tools you need to develop a deeper understanding of general chemistry concepts, the text emphasizes the visual nature of chemistry, illustrating the close interrelationship of the macroscopic, symbolic, and particulate levels of chemistry. The art program illustrates each of these levels in engaging detail--and is fully integrated with key media components. In addition access to OWLv2 may be purchased separately or at a special price if packaged with this text. OWLv2 is an online homework and tutorial system that helps you maximize your study time and improve your success in the course. OWLv2 includes an interactive eBook, as well as hundreds of guided simulations, animations, and video clips. Important Notice: Media content referenced within the product description or the product text may not be available in the ebook version.