Reviews In Computational Chemistry Volume 21

THIS VOLUME, LIKE THOSE PRIOR TO IT, FEATURES CHAPTERS BY EXPERTS IN VARIOUS FIELDS OF COMPUTATIONAL CHEMISTRY. Volume 23 COVERS LINEAR SCALING METHODS FOR QUANTUM CHEMISTRY, VARIATIONAL TRANSITION STATE THEORY, COARSE GRAIN MODELING OF POLYMERS, SUPPORT VECTOR MACHINES, CONICAL INTERSECTIONS, ANALYSIS OF INFORMATION CONTENT USING SHANNON ENTROPY, AND HISTORICAL INSIGHTS INTO HOW COMPUTING EVOLVED IN THE PHARMACEUTICAL INDUSTRY. FROM REVIEWS OF THE SERIES "Reviews in Computational Chemistry remains the most valuable reference to methods and techniques in computational chemistry." —JOURNAL OF MOLECULAR GRAPHICS AND MODELLING "One cannot generally do better than to try to find an appropriate article in the highly successful Reviews in Computational Chemistry. The basic philosophy of the editors seems to be to help the authors produce chapters that are complete, accurate, clear, and accessible to experimentalists (in particular) and other nonspecialists (in general)."

—JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

This volume, like those prior to it, features chapters by experts in various fields of computational chemistry. Topics covered in Volume 18 include molecular modeling, computer-assisted molecular design (camd), quantum chemistry, molecular mechanics and dynamics, and quantitative structure-activity relationships (qsar).

The gap between introductory level textbooks and highly specialized monographs is filled by this modern textbook. It provides in one comprehensive volume the in-depth theoretical background for molecular modeling and detailed descriptions of the applications in chemistry and related fields like drug design, molecular sciences, biomedical, polymer and materials engineering. Special chapters on basic mathematics and the use of respective software tools are included. Numerous numerical examples, exercises and explanatory illustrations as well as a web site with application tools (http://www.amrita.edu/cen/ccmm) support the students and lecturers.

This is the seventh volume in the successful series designed to help the chemistry community keep current with the many new developments in computational techniques. The writing style is refreshingly pedagogical and non-mathematical, allowing students and researchers access to computational methods outside their immediate area of expertise. Each invited author approaches a topic with the aim of

helping the reader understand the material, solve problems, and locate key references quickly.

Theoretical Biochemistry

Reviews in Computational Chemistry, Volume 32

Theories and Models

Theoretical chemistry has been an area of tremendous expansion and development over the past decade; from an approach where we were able to treat only a few atoms quantum mechanically or make fairly crude molecular dynamics simulations, into a discipline with an accuracy and predictive power that has rendered it an essential complementary tool to experiment in basically all areas of science. This volume gives a flavour of the types of problems in biochemistry that theoretical calculations can solve at present, and illustrates the tremendous predictive power these approaches possess. A wide range of computational approaches, from classical MD and Monte Carlo methods, via semi-empirical and DFT approaches on isolated model systems, to Car-Parinello QM-MD and novel hybrid QM/MM studies are covered. The systems investigated also cover a broad range; from membrane-bound proteins to various types of enzymatic reactions as well as inhibitor studies, cofactor properties, solvent effects, transcription and radiation damage to DNA.

THIS VOLUME, WHICH IS DESIGNED FOR STAND-ALONE USE IN TEACHING AND RESEARCH, FOCUSES ON QUANTUM CHEMISTRY, AN AREA OF

SCIENCE THAT MANY CONSIDER TO BE THE CENTRAL CORE OF COMPUTATIONAL CHEMISTRY. TUTORIALS AND REVIEWS COVER * HOW TO OBTAIN SIMPLE CHEMICAL INSIGHT AND CONCEPTS FROM DENSITY FUNCTIONAL THEORY CALCULATIONS, * HOW TO MODEL PHOTOCHEMICAL REACTIONS AND EXCITED STATES, AND * HOW TO COMPUTE ENTHALPIES OF FORMATION OF MOLECULES. A FOURTH CHAPTER TRACES CANADIAN RESEARCH IN THE EVOLUTION OF COMPUTATIONAL CHEMISTRY. ALSO INCLUDED WITH THIS VOLUME IS A SPECIAL TRIBUTE TO QCPE.FROM REVIEWS OF THE SERIES "Reviews in Computational Chemistry proves itself an invaluable resource to the computational chemist. This series has a place in every computational chemist's library."-Journal of the American Chemical Society Volume 6 of the successful series 'Reviews in Computational Chemistry' contains articles of interest to pharmaceutical chemists, biological chemists, chemical engineers, inorganic and organometallic chemists, synthetic organic chemists, polymer chemists, and theoretical chemists. The series is designed to help the chemistry community keep current with the many new developments in computational techniques. The writing style is refreshingly pedagogical and non-mathematical, allowing students and researchers access to computational methods outside their immediate area of expertise.

REVIEWS IN COMPUTATIONAL CHEMISTRY Kenny B. Lipkowitz, Raima Larter, and Thomas R. Cundari This volume, like those prior to it, features chapters by expertsin various fields of computational chemistry. TOPICS COVERED INVolume

21 iNCLUDE AB INITIO QUANTUM SIMULATION IN SOLID STATECHEMISTRY; MOLECULAR QUANTUM SIMILARITY; ENUMERATING MOLECULES;VARIABLE SELECTION; BIOMOLECULAR APPLICATIONS OF POISSON-BOLTZMANNMETHODS; AND DATA SOURCES AND COMPUTATIONAL APPROACHES FORGENERATING MODELS OF GENE REGULATORY NETWORKS. FROM REVIEWS OF THE SERIES "Reviews in Computational Chemistry remains the most valuablereference to methods and techniques in computationalchemistry." --JOURNAL OF MOLECULAR GRAPHICS AND MODELLING "One cannot generally do better than to try to find an appropriatearticle in the highly successful Reviews in ComputationalChemistry. The basic philosophy of the editors seems to be to helpthe authors produce chapters that are complete, accurate, clear,and accessible to experimentalists (in particular) and othernonspecialists (in general)." --JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

Processes and Properties of Biological Systems

Advances in Quantum Chemistry

Simulating Enzyme Reactivity

This volume in the series brings together reknowned experts in the field to present the reader with an account of the latest developments in quantum mechanics, molecular dynamics, and the teaching of computational chemistry. There are so many developments in the field of computational chemistry that it is difficult to keep track of them. The series was established to review the high volume of developments in the field. Rather than create a traditional article,

each author approaches a topic to enable the reader to understand and solve problems and locate key references quickly. Each article has tutorial value. An updated compendium of software for molecular modeling appears as an appendix as in previous volumes. To the editors' knowledge, this is the most complete listing of sources of software for computational chemistry anywhere.

Annual Reports in Computational Chemistry provides timely and critical reviews of important topics in computational chemistry as applied to all chemical disciplines. Topics covered include quantum chemistry, molecular mechanics, force fields, chemical education, and applications in academic and industrial settings. Focusing on the most recent literature and advances in the field, each article covers a specific topic of importance to computational chemists. Quantum chemistry Molecular mechanics Force fields Chemical education and applications in academic and industrial settings

This second volume of the series 'Reviews in Computational Chemistry' explores new applications, new methodologies, and new perspectives. The topics covered include conformational analysis, protein folding, force field parameterizations, hydrogen bonding, charge distributions, electrostatic potentials, electronic spectroscopy, molecular property correlations, and the computational chemistry literature. Methodologies described include conformational search strategies, distance geometry, molecular mechanics, molecular dynamics, ab initio and semiempirical molecular orbital calculations, and quantitative structure-activity relationships (QSAR) using topological and electronic descriptors. A compendium of molecular modeling software will help users select the computational tools they need. Each chapter in 'Reviews in Computational Chemistry' serves as a brief tutorial for organic, physical,

pharmaceutical, and biological chemists new to the field. Practitioners will be interested in the recent advances.

This book is an account of current developments in computational chemistry, a new multidisciplinary area of research. Experts in computational chemistry, the editors use and develop techniques for computer-assisted molecular design. The core of the text itself deals with techniques for computer-assisted molecular design. The book is suitable for both beginners and experts. In addition, protocols and software for molecular recognition and the relationship between structure and biological activity of drug molecules are discussed in detail. Each chapter includes a mini-tutorial, as well as discussion of advanced topics. Special Feature: The appendix to this book contains an extensive list of available software for molecular modeling.

Computational Chemistry

Essentials of Computational Chemistry

Theoretical Aspects of Chemical Reactivity

Essentials of Computational Chemistry provides a balanced introduction to this dynamic subject. Suitable for both experimentalists and theorists, a wide range of samples and applications are included drawn from all key areas. The book carefully leads the reader thorough the necessary equations providing information explanations and reasoning where necessary and firmly placing each equation in context.

The Reviews in Computational Chemistry series brings together leading authorities in the field to teach the newcomer and update the expert on topics centered on molecular

modeling, such as computer-assisted molecular design (CAMD), quantum chemistry, molecular mechanics and dynamics, and quantitative structure-activity relationships (QSAR). This volume, like those prior to it, features chapters by experts in various fields of computational chemistry. Topics in Volume 29 include: Noncovalent Interactions in Density-Functional Theory Long-Range Inter-Particle Interactions: Insights from Molecular Quantum Electrodynamics (QED) Theory Efficient Transition-State Modeling using Molecular Mechanics Force Fields for the Everyday Chemist Machine Learning in Materials Science: Recent Progress and Emerging Applications Discovering New Materials via a priori Crystal Structure Prediction Introduction to Maximally Localized Wannier Functions Methods for a Rapid and Automated Description of Proteins: Protein Structure, Protein Similarity, and Protein Folding

THIS BOOK HAS SIX TUTORIALS AND REVIEWS WRITTEN BY INVITED EXPERTS. FIVE CHAPTERS TEACH TOPICS IN QUANTUM MECHANICS AND MOLECULAR SIMULATIONS. THE SIXTH CHAPTER EXPLAINS HOW PROGRAMS FOR CHEMICAL STRUCTURE DRAWING WORK. AN EDITORIAL DISCUSSES SOME OF THE MOST WELL-KNOWN PERSONAGES IN COMPUTATIONAL CHEMISTRY. FROM REVIEWS OF THE SERIES "Anyone who is doing or intends to do computational research on molecular structure and design should seriously consider purchasing this book for his or her personal library."-JOURNAL OF COMPUTATIONAL CHEMISTRY. "These reviews are becoming regarded as the standard reference

among both specialists and novices in the expanding field of computational chemistry." -JOURNAL OF MOLECULAR GRAPHICS AND MODELLING. "[This book is] written for newcomers learning about molecular modeling techniques as well as for seasoned professionals who need to acquire expertise in areas outside their own."-JOURNAL OF CHEMICAL INFORMATION AND COMPUTER SCIENCE.

The Reviews in Computational Chemistry series brings together leading authorities in the field to teach the newcomer and update the expert on topics centered on molecular modeling, such as computer-assisted molecular design (CAMD), quantum chemistry, molecular mechanics and dynamics, and quantitative structure-activity relationships (QSAR). This volume, like those prior to it, features chapters by experts in various fields of computational chemistry. Topics in Volume 31 include: Lattice-Boltzmann Modeling of Multicomponent Systems: An Introduction Modeling Mechanochemistry from First Principles Mapping Energy Transport Networks in Proteins The Role of Computations in Catalysis The Construction of Ab Initio Based Potential Energy Surfaces Uncertainty Quantification for Molecular Dynamics

Recent Advances in Computational Quantum Chemistry

Reviews in Computational Chemistry

Computational Methods in Enzyme Catalysis

Theoretical Aspects of Chemical Reactivity provides a broad overview of recent theoretical and computational advancements in the field of

chemical reactivity. Contributions have been made by a number of leaders in the field covering theoretical developments to applications in molecular systems and clusters. With an increase in the use of reactivity descriptors, and fundamental theoretical aspects becoming more challenging, this volume serves as an interesting overview where traditional concepts are revisited and explored from new viewpoints, and new varieties of reactivity descriptors are proposed. Includes applications in the frontiers of reactivity principles, and introduces dynamic and statistical viewpoints to chemical reactivity and challenging traditional concepts such as aromaticity. * Written by specialists in the field of chemical reactivity * An authoritative overview of the research and progress * An essential reference material for students
Annual Reports in Computational Chemistry is a new periodical providing timely and critical reviews of important topics in computational chemistry as applied to all chemical disciplines. Topics covered include quantum chemistry, molecular mechanics, force fields, chemical education, and applications in academic and industrial settings. Each volume is organized into (thematic) sections with contributions written by experts. Focusing on the most recent literature and advances in the field, each article covers a specific topic of importance to computational chemists. Annual

Reports in Computational Chemistry is a 'must' for researchers and students wishing to stay up-to-date on current developments in computational chemistry. * Broad coverage of computational chemistry and up-to-date information * The topics covered include quantum chemistry, molecular mechanics, force fields, chemical education, and applications in academic and industrial settings * Each chapter reviews the most recent literature on a specific topic of interest to computational chemists

Computational Quantum Chemistry presents computational electronic structure theory as practised in terms of ab initio waveform methods and density functional approaches. Getting a full grasp of the field can often prove difficult, since essential topics fall outside of the scope of conventional chemistry education. This professional reference book provides a comprehensive introduction to the field. Postgraduate students and experienced researchers alike will appreciate Joseph McDouall's engaging writing style. The book is divided into five chapters, each providing a major aspect of the field. Electronic structure methods, the computation of molecular properties, methods for analysing the output from computations and the importance of relativistic effects on molecular properties are also discussed. Links to the websites of widely used software packages are provided so that the reader can gain first hand

experience of using the techniques described in the book. Dr McDouall has more than 25 years experience in theoretical chemistry; as a reader at the University of Manchester his research interests include the application of quantum chemical methods to the elucidation of chemical problems and the development and implementation of electronic structure methods that permit the accurate prediction of chemical structures and molecular properties.

Computational chemistry has become extremely important in the last decade, being widely used in academic and industrial research. Yet there have been few books designed to teach the subject to nonspecialists. Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics is an invaluable tool for teaching and researchers alike. The book provides an overview of the field, explains the basic underlying theory at a meaningful level that is not beyond beginners, and it gives numerous comparisons of different methods with one another and with experiment. The following concepts are illustrated and their possibilities and limitations are given: - potential energy surfaces; - simple and extended Hückel methods; - ab initio, AM1 and related semiempirical methods; - density functional theory (DFT). Topics are placed in a historical context, adding interest to them and removing much of their apparently arbitrary aspect. The large number of

references, to all significant topics mentioned, should make this book useful not only to undergraduates but also to graduate students and academic and industrial researchers.

Introduction to the Theory and Applications of Molecular and Quantum Mechanics

Computational Chemistry and Molecular Modeling

Computational Quantum Chemistry

Advances in Quantum Chemistry publishes surveys of current developments in the rapidly developing field of quantum chemistry--a field that falls between the historically established areas of mathematics, physics,chemistry, and biology. With invited reviews written by leading international researchers, each presenting new results, this quality serial provides a single vehicle for following progress in this interdisciplinary area. "Volume 28 collects papers written in honor of Geerd H.F. Diercksen. Diercksen is a pioneer in the field of quantum mechanics whose research includes studies of the structure and stability of hydrogen-bonded and Van der Waals dimers and small clusters, thevibrational and rotational spectra of diatomic and

triatomic molecules, on static electric properties in solutions and of molecules absorbed on surfaces. His results are essential in molecular and atomic physics, in astrophysics, and in biochemistry.

FROM REVIEWS OF THE SERIES "Reviews in Computational Chemistry remains the most valuable reference to methods and techniques in computational chemistry." -JOURNAL OF MOLECULAR GRAPHICS AND MODELLING "One cannot generally do better than to try to find an appropriate article in the highly successful Reviews in Computational Chemistry. The basic philosophy of the editors seems to be to help the authors produce chapters that are complete, accurate, clear, and accessible to experimentalists (in particular) and other nonspecialists (in general)." -JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

The present status of Density Functional Theory (DFT), which has evolved as the main technique for the study of matter at the atomistic level, is described in this volume. Knowing the behavior of atoms and molecules provides a sure avenue

for the design of new materials with specific features and properties in many areas of science and technology. A technique based on purely first principles allowing large savings in time and money greatly benefits the specialist or designer of new materials. The range of areas where DFT is applied has expanded and continues to do so. Any area where a molecular system is the center of attention can be studied using DFT.The scope of the 22 chapters in this book amply testifies to this.

The first volume of this two part series is concerned with the fundamental aspects of relativistic quantum theory, outlining the enormous progress made in the last twenty years in this field. The aim was to create a book such that researchers who become interested in this exciting new field find it useful as a textbook, and do not have to rely on a rather large number of specialized papers published in this area. · No title is currently available that deals with new developments in relativistic quantum electronic structure theory · Interesting and relevant to graduate students in

chemistry and physics as well as to all researchers in the field of quantum chemistry · As treatment of heavy elements becomes more important, there will be a constant demand for this title

Recent Developments and Applications of Modern Density Functional Theory

Relativistic Electronic Structure Theory - Fundamentals

Molecular Structure and Properties in Silico

Computational chemistry is increasingly used in conjunction with organic, inorganic, medicinal, biological, physical, and analytical chemistry, biotechnology, materials science, and chemical physics. This series is essential in keeping those individuals involved in these fields abreast of recent developments in computational chemistry.

This series is reviewing advances in the rapidly growing and evolving field of computational chemistry. It was established to keep track of the many new developments and is therefore providing a valuable service to the scientific community.

Not only a major reference work for sale to the library market, Reviews in Computational Chemistry is now a purchase by individuals due to the

explosive growth in the use of computational chemistry throughout many scientific disciplines. In an instructional and nonmathematical style, these books provide an access to computational methods often outside a researcher's area of expertise. Volumes 9 & 10 represent the next two volumes in the successful series designed to help the chemistry community keep current with the many new developments in computational techniques. Many chapters are written as tutorials to introduce the many facets of computational chemistry, including molecular modeling, computer-assisted molecular design (CAMD), quantum chemistry, molecular mechanics and dynamics, and quantitative structure-activity relationships (QSAR). The authors provide necessary background and theory, strategies for implementing the methods, pitfalls to avoid, applications, and references. The Reviews in Computational Chemistry series bringstogether leading authorities in the field. The chapters in thisbook series are written to teach the newcomer and update theexpert. Topics include computational chemistry, molecular modeling,computer-assisted molecular design (CAMD), quantum chemistry,molecular mechanics and dynamics, and quantitativestructure-activity relationships (QSAR). Detailed author and subject indices on each volume help thereader to quickly discover particular topics. The chapters are approached in a tutorial manner and written ina non-

mathematical style allowing students and researchers toaccess computational methods outside their immediate area ofexpertise.

Annual Reports in Computational Chemistry

Volume 11

Principles and Applications

The simulation of enzymatic processes is a well-established field within computational chemistry, as demonstrated by the 2013 Nobel Prize in Chemistry. It has been attracting increasing attention in recent years due to the potential applications in the development of new drugs or new environmental-friendly catalysts. Featuring contributions from renowned authors, including Nobel Laureate Arieh Warshel, this book explores the theories, methodologies and applications in simulations of enzyme reactions. It is the first book offering a comprehensive perspective of the field by examining several different methodological approaches and discussing their applicability and limitations. The book provides the basic knowledge for postgraduate students and researchers in chemistry, biochemistry and biophysics, who want a deeper understanding of complex biological process at the molecular level.

VOLUME 12 REVIEWS IN COMPUTATIONAL CHEMISTRY Kenny B. Lipkowitz and Donald B. Boyd HOW DOES ONE COMPUTE FREE ENERGY AND ENTROPY FROM MOLECULAR SIMULATIONS? WHAT HAPPENS WHEN SIMULATIONS ARE RUN WITH CONSTRAINTS? HOW SHOULD SIMULATIONS BE PERFORMED TO MODEL

INTERFACIAL PHENOMENA? HOW IS DENSITY FUNCTIONAL THEORY USED TO SIMULATE MATERIALS? WHAT QUANTUM MECHANICAL METHODS SHOULD BE USED TO COMPUTE NONLINEAR OPTICAL PROPERTIES OF MATERIALS? WHICH PARAMETERS ARE MOST INFLUENTIAL IN A MOLECULAR SIMULATION? HOW CAN CRYSTAL STRUCTURES BE PREDICTED? TUTORIALS PROVIDING ANSWERS TO THESE QUESTIONS ARE THE FOCUS OF THIS BOOK. FROM REVIEWS OF THE SERIES "The series continues to be one of the most useful information sources." -JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

REVIEWS IN COMPUTATIONAL CHEMISTRY THE LATEST VOLUME IN THE REVIEWS IN COMPUTATIONAL CHEMISTRY SERIES, THE INVALUABLE REFERENCE TO METHODS AND TECHNIQUES IN COMPUTATIONAL CHEMISTRY

Reviews in Computational Chemistry reference texts assist researchers in selecting and applying new computational chemistry methods to their own research. Bringing together writings from leading experts in various fields of computational chemistry, Volume 32 covers topics including global structure optimization, time-dependent density functional tight binding calculations, non-equilibrium self-assembly, cluster prediction, and molecular simulations of microphase formers and deep eutectic solvents. In keeping with previous books in the series, Volume 32 uses a non-mathematical style and tutorial-based approach that provides students and researchers with easy access to computational methods outside their area of expertise. The chapters comprising Volume 32 are connected by two themes: methods that can be

broadly applied to a variety of systems, and special considerations required when modeling specific system types. Each in-depth chapter contains background and theory, strategies for using the methods correctly, mini-tutorials and best practices, and critical literature reviews highlighting advanced applications. Essential reading for both newcomers and experts in the area of molecular modeling, this state-of-the-art resource: Covers topics such as non-deterministic global optimization (NDGO) approaches and excited-state dynamics calculations Contains a detailed overview of deep eutectic solvents (DESs) and simulation methods Presents methodologies for investigating chemical systems that form microphases with periodic morphologies such as lamellae and cylinders Features step-by-step tutorials on applying techniques to probe and understand the chemical dynamics exhibited in a system Includes detailed subject indices on each volume in the series and up-to-date compendiums of molecular modeling software, services, programs, suppliers, and other useful information Reviews in Computational Chemistry, Volume 32 is a must-have guide for computational chemists, theoretical chemists, pharmaceutical chemists, biological chemists, chemical engineers, researchers in academia and industry, and graduate students involved in molecular modeling.

From reviews of the series: 'Many of the articles are indeed accessible to any interested nonspecialist, even without theoretical background.' Journal of the American Chemical Society '...an invaluable resource for the serious molecular modeler.' Chemical Design Automation News

This volume in computational chemistry includes aspects of: theoretical chemistry, physical chemistry, computer graphics in chemistry, molecular structure, and pharmaceutical chemistry.

The Reviews in Computational Chemistry series brings together leading authorities in the field to teach the newcomer and update the expert on topics centered on molecular modeling. • Provides background and theory, strategies for using the methods correctly, pitfalls to avoid, applications, and references • Contains updated and comprehensive compendiums of molecular modeling software that list hundreds of programs, services, suppliers and other information that every chemist will find useful • Includes detailed indices on each volume help the reader to quickly discover particular topics • Uses a tutorial manner and non-mathematical style, allowing students and researchers to access computational methods outside their immediate area of expertise

Not only a major reference work for sale to the library market, this series is now receiving an increase in purchases by individuals. This increase is due to the explosive growth in the use of computational chemistry throughout many scientific disciplines As each volume does not follow a singular theme, the table of contents is a vital tool in the defining the areas examined by a volume

The series contains updated and comprehensive compendiums of molecular modeling software that list hundreds of programs, services, suppliers, and other information that every chemist will find useful Detailed author and subject indices on each volume help the reader to quickly discover particular topics Uniting the most respected authors in their fields, the series is designed to help the reader stay abreast of the many new developments in computational techniques The chapters are approached in a tutorial manner and wirtten in a non-mathematical style allowing students and researches to access computational methods outside their immediate area of expertise
The Reviews in Computational Chemistry series brings together leading authorities in the field to teach the newcomer and update the expert on topics centered around molecular modeling, such as computer-assisted molecular design (CAMD), quantum chemistry, molecular mechanics and dynamics, and quantitative structure-activity relationships (QSAR). This volume, like those prior to it, features chapters by experts in various fields of computational chemistry. Topics in Volume 28 include: Free-energy Calculations with Metadynamics Polarizable Force Fields for Biomolecular Modeling Modeling Protein Folding Pathways Assessing Structural Predictions of Protein-Protein Recognition Kinetic Monte Carlo Simulation of Electrochemical Systems

Reactivity and Dynamics at Liquid Interfaces

Computational chemistry is increasingly used in most areas ofmolecular science including organic, inorganic, medicinal,biological, physical, and analytical chemistry. Researchers inthese fields who do molecular modelling need to understand and staycurrent with recent developments. This volume, like those prior toit, features chapters by experts in various fields of computationalchemistry. Two chapters focus on molecular docking, one of whichrelates to drug discovery and cheminformatics and the other toproteomics. In addition, this volume contains tutorials onspin-orbit coupling and cellular automata modeling, as well as anextensive bibliography of computational chemistry books. FROM REVIEWS OF THE SERIES "Reviews in Computational Chemistryremains the most valuable reference to methods and techniques incomputational chemistry."—JOURNAL OF MOLECULAR GRAPHICS ANDMODELLING "One cannot generally do better than to try to find anappropriate article in the highly

successful Reviews inComputational Chemistry. The basic philosophy of the editors seemsto be to help the authors produce chapters that are complete,accurate, clear, and accessible to experimentalists (in particular)and other nonspecialists (in general)."—JOURNAL OF THEAMERICAN CHEMICAL SOCIETY