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There are strong indications that, in the 21st century, computational chemistry will be a prime research tool not only for the basic sciences but also for the life and

materials sciences. Recent developments in nanotechnology allow us to detect a layer of single atoms. Researchers are able not only to image but also to manipulate molecules and atoms. It does not take much imagination to realize that before performing such a task on a real system it is much easier and faster to study models on computers. That is the aim of this volume — it provides up-to-date reviews which cover representative areas of computational chemistry. In Chapter 1, Y Ishikawa and M J Vilkas provide a review of multireference Moller–Plesset (MR–MP) perturbation theory. Fifteen years ago Roberto Car of Princeton University and Michele Parrinello of Max Planck Institute introduced a method that revolutionized electronic structure calculations for molecules, liquids and solids. Ursula Rothlisberger, a former member of Parrinello's group, reviews the formation of the method in its most common implementations in Chapter 2. In the third chapter, Isaac B Bersuker describes the general theory of the combined quantum mechanics–molecular mechanics (QM/MM) approach. In Chapter 4, Marcel Allavena and David White present a review of applications of computational chemistry to proton transfer, the primary process for acid-base chemistry on zeolites. Chapter 5 is a review by S Roszak and J Leszczynski of recent data on the clusters formed from the charged ion and weakly interacting ligands. The last chapter, contributed by Carlos R Handy, is devoted to recent developments in the incorporation of continuous wavelet transform analysis into quantum operator theory. Contents:Relativistic Multireference Møller–Plesset Perturbation Theory (Y Ishikawa & M J Vilkas)15 Years of Car–Parrinello Simulations in Physics, Chemistry and

Biology (U Rothlisberger)Methods of Combined Quantum/Classical (QM/MM) Modeling for Large Organometallic and Metallobiochemical Systems (I B Bersuker)A Review of Ab Initio Calculations on Proton Transfer in Zeolites (M Allavena & D White)Ionic Clusters with Weakly Interacting Components–Magic Numbers Rationalized by the Shell Structure (S Roszak & J Leszczynski)Turning Point Quantization and Scalet–Wavelet Analysis (C R Handy) Readership: Graduate students and researchers in computational chemistry. Keywords:Computational Chemistry;Combined Quantum/Classical Methods;QM/MM Methods;Fragmentary Calculations;Quantum/Classical Charge Transfer;Transition Metal Systems;Metallobiochemical Systems;Organometallic Systems;Picket-Fence Porphyrin;Vitamin B12Reviews:“… it certainly deserves a spot in chemistry libraries. Overall, the reviews are well-done, and if one of them matches a field of work that a researcher plans to enter, it will save a great deal of library exploration.”Journal of the American Chemical Society

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

THIS VOLUME, LIKE THOSE PRIOR TO IT, FEATURES CHAPTERS BY EXPERTSIN VARIOUS FIELDS OF COMPUTATIONAL CHEMISTRY. TOPICS COVERED INVOLUME 20 INCLUDE VALENCE THEORY, ITS HISTORY, FUNDAMENTALS, ANDAPPLICATIONS; MODELING OF SPIN-FORBIDDEN REACTIONS; CALCULATION OFTHE ELECTRONIC SPECTRA OF LARGE MOLECULES; SIMULATING CHEMICALWAVES AND PATTERNS; FUZZY SOFT-COMPUTING METHODS AND THEIRAPPLICATIONS IN CHEMISTRY; AND DEVELOPMENT OF COMPUTATIONAL MODELSFOR ENZYMES, TRANSPORTERS, CHANNELS, AND RECEPTORS RELEVANT TOADME/TOX. FROM REVIEWS OF THE SERIES "Reviews in Computational Chemistry remains the most valuablereference to methods and techniques in computationalchemistry." -JOURNAL OF MOLECULAR GRAPHICS AND MODELING "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

Chaired by K Wüthrich (Nobel Laureate in Chemistry, 2002) and co-chaired by B Weckhuysen, this by-invitation-only conference has gathered 39 participants — who are leaders in the field of computational modeling and its applications in Chemistry, Material Sciences and Biology. Highlights of the Conference Proceedings are short, prepared statements by all the participants and the records of lively discussions on the current and future perspectives in the field of computational modeling, from chemistry to materials to biology.

Detailed study of the rates and mechanisms of combustion reactions has not been in the mainstream of combustion research until the recent recognition that further progress in optimizing burner performance and reducing pollutant emission can only be done with fundamental understanding of combustion chemistry. This has become apparent at a time when our understanding of the chemistry, at least of small-molecule combustion, and our ability to model combustion processes on large computers have developed to the point that real confidence can be placed in the results. This book is an introduction for outsiders or beginners as well as a reference work for people already active in the field. Because the spectrum of combustion scientists ranges from chemists with little computing experience to engineers who have had only one college chemistry course, everything needed to bring all kinds of beginners up to the level of current practice in detailed

combustion modeling is included. It was a temptation to include critical discussions of modeling results and computer programs that would enable outsiders to start quickly into problem solving. We elected not to do either, because we feel that the former are better put into the primary research literature and that people who are going to do combustion modeling should either write their own programs or collaborate with experts. The only exception to this is in the thermochemical area, where programs have been included to do routine fitting operations. For reference purposes there are tables of thermochemical, transport-property, and rate coefficient data.

This book presents an overview of recent progress in computational techniques as well as examples of the application of existing computational methods in different areas of chemistry, physics, and biochemistry. Introductory chapters cover a broad range of fundamental topics, including: state-of-the-art basis set expansion methods for computing atomic and molecular electronic structures based on the use of relativistic quantum mechanics; the most recent developments in Hartree-Fock methods, particularly in techniques suited for very large systems; the current analysis of the solute-solvent free energy of interaction and the physical bases used to evaluate the electrostatic, cavitation, and dispersion terms; an introduction to the additive fuzzy electron density fragmentation scheme within various ab initio Hartree-Fock quantum-chemical computational schemes, which has provided the means for generating representative molecular fragment densities

characteristic to their local environment within a molecule. This book also features a review of recent ab initio calculations on the structure and interactions of DNA bases, a chapter on computational approaches to the design of safer drugs and their molecular properties, and a systematic conceptual study on a route which allows one to stuff fullerenes.

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.

Practical Aspects of Computational Chemistry II: An Overview of the Last Two Decades and Current Trends gathers the discussion of advances made within the last 20 years by well-known experts in the area of theoretical and computational chemistry and physics. The title reflects the celebration of the twentieth

anniversary of the “Conference on Current Trends in Computational Chemistry (CCTCC)” to success of which all authors contributed. Starting with the recent development of modeling of solvation effect using the Polarizable Continuum Model (PCM) at the Coupled-Cluster level and the effects of extreme pressure on the molecular properties within the PCM framework, this volume focuses on the association/dissociation of ion pairs in binary solvent mixtures, application of graph theory to determine the all possible structures and temperature-dependent distribution of water cluster, generalized-ensemble algorithms for the complex molecular simulation, QM/MD based investigation of formation of different nanostructures under nonequilibrium conditions, quantum mechanical study of chemical reactivity of carbon nanotube, covalent functionalization of single walled-carbon nanotube, designing of functional materials, importance of long-range dispersion interaction to study nanomaterials, recent advances in QSPR/QSAR analysis of nitrocompounds, prediction of physico-chemical properties of energetic materials, electronic structure and properties of 3d transition metal dimers, the s-bond activation reactions by transition metal complexes, theoretical modeling of environmental mercury depletion reaction, organolithium chemistry and computational modeling of low-energy electron induced DNA damage. Practical Aspects of Computational Chemistry II: An Overview of the Last Two Decades and Current Trends is aimed at theoretical and computational chemists, physical chemists, materials scientists, and particularly those who are eager to apply computational chemistry methods to problems of chemical and physical

importance. This book provides valuable information to undergraduate, graduate, and PhD students as well as to established researchers. Practical Aspects of Computational Chemistry II: An Overview of the Last Two Decades and Current Trends is aimed at theoretical and computational chemists, physical chemists, materials scientists, and particularly those who are eager to apply computational chemistry methods to problems of chemical and physical importance. This book provides valuable information to undergraduate, graduate, and PhD students as well as to established researchers.