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Vast progress in the area of computational chemistry has been achieved in the last decade of the 20th century. Theoretical methods such as quantum mechanics, molecular dynamics and statistical mechanics have been successfully used to characterize chemical systems and to design new materials, drugs and chemicals. With this in mind, the contributions to this volume were collected. The contributions include predictions of the transport properties of molecular structures at the atomic level, which is of importance in solving crucial technological problems such as electromigration or temperature and statistical effects. Although currently restricted to calculation of systems containing no more than a few thousand atoms, nonempirical (ab initio) quantum chemical methods are quickly gaining popularity among researchers investigating various aspects of biological systems. The development of efficient methods for application to large molecular systems is the focus of two chapters. They include an overview of development and applications of parallel and order-N Density Functional Theory (DFT) methods and the development of new methods for calculation of electron dynamical correlation for large molecular systems. For small and medium-sized molecules, chemical accuracy of quantum chemical predictions has already been achieved in many fields of application. Among the most accurate methods are Coupled Cluster (CC) approaches, but their accuracy comes at a price — such methodologies are among the most computationally demanding. Two chapters review approximate strategies developed to include triple excitations within the coupled cluster and the performance of the explicitly correlated CC method based on the so-called R12 ansatz. The Quantum Molecular Dynamics (QMD) approach has revolutionized electronic structure calculations for molecular reactions. The last chapter of the volume provides details of QMD studies on interconversion of nitronium ions and nitric acid in small water clusters. Contents:Molecules as Components in Electronic Devices: A First-Principles Study (M Di Ventra)Tackling DNA with Density Functional Theory: Development and Application of Parallel and Order-N DFT Methods (C F Guerra et al.)Low-Scaling Methods for Electron Correlation (S Saebø)Iterative and Non-Iterative Inclusion of Connected Triple Excitations in Coupled-Cluster Methods: Theory and Numerical Comparisons for Some Difficult Examples (J D Watts)Explicitly Correlated Coupled Cluster R12 Calculations (J Noga & P Valiron)Ab Initio Direct Molecular Dynamics Studies of Atmospheric Reactions: Interconversion of Nitronium Ions and Nitric Acid in Small Clusters (Y Ishikawa & R C Binning, Jr.) Readership: Graduate students and researchers in computational, theoretical and quantum chemistry. Keywords: Excerpts from and citations to reviews of more than 8,000 books each year, drawn from coverage of 109 publications. Book Review Digest provides citations to and excerpts of reviews of current juvenile and adult fiction and nonfiction in the English language. Reviews of the following types of books are excluded: government publications, textbooks, and technical books in the sciences and law. Reviews of books on science for the general reader, however, are included. The reviews originate in a group of selected periodicals in the humanities, social sciences, and general science published in the United States, Canada, and Great Britain. - Publisher. The gap between experimental objects and models for calculations in chemistry is being bridged. The size of experimental nano-objects is decreasing, while reliable calculations are feasible for larger and larger molecular systems. The results of these calculations for isolated molecules are becoming more relevant for experiments. However, there are still significant challenges for computational methods. This series of books presents reviews of current advances in computational methodologies and applications. Chapter 1 of this volume provides an overview of the theoretical and numerical aspects in the development of the polarizable continuum model (PCM). Chapter 2 demonstrates a multiplicative scheme used to estimate the properties of two- and three-dimensional clusters from the properties of their one-dimensional components. Chapter 3 discusses the application of ab initio methods for a reliable evaluation of the characteristics of hydrogen-bonded and van der Waals complexes. Ab initio quantum-chemical methods are popular among researchers investigating various aspects of DNA. The properties of DNA base polyads linked by base-base hydrogen bonds are reviewed in Chapter 4, while Chapter 5 reviews the primary radiation-induced defects in nucleic acid building blocks, and how DNA can be influenced by chemical and environmental effects. Finally, Chapter 6 discusses available experimental data of DNA bases, base pairs, and their complexes with water. Contents:Computational Modelling of the Solvent Effects on Molecular Properties: An Overview of the Polarizable Continuum Model (PCM) Approach (R Cammi et al.)Electronic and Nonlinear Optical Properties of 2-Methyl-4-Nitroaniline Clusters (M Guillaume et al.)Ab Initio Calculations of the Intermolecular Nuclear Spin-Spin Coupling Constants (M Pecul & J Sadlej)Base Polyad Motifs in Nucleic Acids — Biological Significance, Occurrence in Three-Dimensional Experimental Structures and Computational Studies (M Meyer & J Sühnel)Model Calculations of Radiation Induced Damage in DNA Constituents Using Density Functional Theory (D M Close)Excited States of Nucleic Acid Bases (M K Shukla & J Leszczynski) Readership: Graduate students and researchers in computational chemistry. Keywords:Computational Chemistry A two-time AJN Book of the Year Award winner and a 2013 Doody Core Title! This distinguished text provides top-tier guidance for advanced practice nurses on how to perform a comprehensive systematic review of available research to inform scholarly work, particularly in DNP and PhD programs. With a strategic focus on the search process and assessing the quality of the evidence, this text presents, clearly and comprehensively, all of the knowledge and skills necessary to conduct a foundational CSR in eight concrete steps. This text examines how to write a CSR proposal, final report, and a policy brief based on systematic review findings. Two finished proposals and two completed systematic reviews demonstrate each step of the process from start to finish. Additionally, the text covers software used in research queries and provides helpful strategies for effectively using the search function when seeking information. The Third Edition offers four new chapters with incisive recommendations for performing a CSR and addressing new ways CSR is being implemented in today's healthcare environment. It describes the latest methodological advances, including living systematic reviews and dominance scores for economic review. Two complete CSRs along with new and updated examples throughout the book further aid readers in their pursuit of excellence in scholarly work. New to the Third Edition: New Chapters: How to choose the right critical appraisal tool Writing the final report and disseminating the results of systematic reviews Disseminating results with how to write a policy brief and/or press release on CSR results Example of a meta-analysis using GRADE Offers increased focus on dissemination Includes new and updated examples reflecting latest trends in nursing scholarly work Key Features: Provides the knowledge and skills necessary to conduct a CSR from start to finish Teaches readers how to conduct high-quality systematic reviews Instructs readers on pertinent resources and methods for optimal library-related systematic review research efforts Describes how to best search research databases to facilitate scholarly work Includes objectives, summary points, end-of-chapter exercises, discussion questions, suggested reading, and references to enhance understanding Offering complete, up-to-date coverage of everything from basic science through current clinical practice, Hall Anesthesia: A Comprehensive Review, 6th Edition, provides 1,000 review questions that help you improve your mastery of anesthesiology. You'll reinforce your current knowledge, identify areas that require more study, and improve your long-term retention of the material - all while preparing for certification and re-certification examinations as well as clinical practice. Provides 1,000 completely updated review questions (more than 100 are brand-new) with explanations in the answers. Every question has been reviewed by at least one additional author and vetted by Mayo residents to ensure a consistent level of difficulty. Familiarizes you with the current ABA exam content and format, with challenging board review questions and answers covering the latest discoveries and techniques in physics, biochemistry, and anesthesia equipment; the newest drugs and drug categories; and the most recent information on all anesthesia subspecialties. Allows you to test interactively online with a scoreboard and notes field. Offers discussions after each question, along with corresponding page references to major anesthesia texts so it's easy to find more information on any subject. Enhanced eBook version included with purchase, which allows you to access all of the text, figures, and references from the book on a variety of devices Say goodbye to top-down evaluations and hello to collaboration and change! How can you leverage the objectivity of outside evaluators and the knowledge of local educators who understand your school's particular situation to help you drive school improvement? The answer: collaborative schools reviews conducted by personnel from within your district in collaboration with your school leadership team. Here you'll find: A research-based case for the value and results of collaborative school reviews Best practices for creating review teams, conducting onsite classroom observations, and aligning with district goals How-to's for effectively using data to gain a balanced view of school performance This volume presents a balanced blend of methodological and applied contributions. It supplements well the first three volumes of the series, revealing results of current research in computational chemistry. It also reviews the topographical features of several molecular scalar fields. A brief discussion of topographical concepts is followed by examples of their application to several branches of chemistry. The size of a basis set applied in a calculation determines the amount of computer resources necessary for a particular task. The details of a common strategy — the ab initio model potential method — which could be used to minimize such a task are revealed in the subsequent contribution. Such an approach is applied to atoms, molecules and solids. Two chapters are devoted to the prediction of solvent effects in biological systems. These effects are significant for interactions of nucleic acid bases and crucial for an evaluation of the free energies that govern the associations of macromolecules in aqueous solutions. A chapter on the developments and applications of the multireference Moller–Plesset method could be used as a reference in theoretical studies of systems where both the dynamical and nondynamical correlation effects should be accounted for. This technique is an efficient tool in such investigations. An explosive application of computational techniques — studies of detonation initiation and sensitivity in energetic compounds — is discussed in detail in the last chapter. The computational treatment of such unstable compounds allows the prediction of their crucial properties without being subject to their destructive forces. Contents:Topography of Atomic and Molecular Scalar Fields (S R Gadre)The Ab Initio Model Potential Method: A Common Strategy for Effective Core Potential and Embedded Cluster Calculations (L Seijo & Z Barandiaran)Continuum Models of Macromolecular Association in Aqueous Solution (M A Olson)Interactions of Nucleic Acid Bases: The Role of Solvent (M Orozco et al.)Recent Advances in Multireference Møller–Plesset Method (K Hirao et al.)Detonation Initiation and Sensitivity in Energetic Compounds: Some Computational Treatments (P Politzer & H E Alper) Readership: Graduate students and researchers in computational chemistry. Keywords:Continuum Model;Protein-Protein Association;Protein-Nucleic Acid Binding;Free Energy of Complex Formation;Molecular Recognition;Poisson-Boltzmann Equation;Dielectric Models;Solvation;Hydrophobic Effect;Protein Reorganization;ECP;AIMP;Core Potential;Embedding Potential;Model Potential;Ab Initio;Embedded Cluster;Relativistic;Impurity;Doped Crystal How envy, spite, and the pursuit of admiration influence politics Why do governments underspend on policies that would make their constituents better off? Why do people participate in contentious politics when they could reap benefits if they were to abstain? In Envy in Politics, Gwyneth McClendon contends that if we want to understand these and other forms of puzzling political behavior, we should pay attention to envy, spite, and the pursuit of admiration--all manifestations of our desire to maintain or enhance our status within groups. Drawing together insights from political philosophy, behavioral economics, psychology, and anthropology, McClendon explores how and under what conditions status motivations influence politics. Through surveys, case studies, interviews, and an experiment, McClendon argues that when concerns about in-group status are unmanaged by social conventions or are explicitly primed by elites, status motivations can become drivers of public opinion and political participation. McClendon focuses on the United States and South Africa—two countries that provide tough tests for her arguments while also demonstrating that the arguments apply in different contexts. From debates over redistribution to the mobilization of collective action, Envy in Politics presents the first theoretical and empirical investigation of the connection between status motivations and political behavior. ' Vast progress in the area of computational chemistry has been achieved in the last decade. Theoretical methods such as quantum mechanics, molecular dynamics and statistical mechanics have been successfully used to characterize chemical systems and to design new materials, drugs and chemicals. The reviews presented in this volume discuss the current advances in computational methodologies and their applications. The areas covered include materials science, nanotechnology, inorganic and biological systems. The major thrust of the book is to bring timely overviews of new findings and methods applied in the rapidly changing field of computational chemistry. Contents:Molecular Electronics with Gaussian98/03 (J J Palacios et al.)Molecular Dynamics Simulations of Single Molecule Atomic Force Microscope Experiments (W Nowak & P E Marszalek)Molecular Dynamics Simulations of a Molecular Electronics Device: The NanoCell (J Seminario et al.)Computation of Excited State Potential Energy Surfaces via Linear Response Theories Based on State Specific Multi-Reference Coupled Electron-Pair Approximation Like Methods (S Chattopadhyay et al.)Modelling of Anisotropic Exchange Coupling in Rare-Earth–Transition-Metal Pairs: Applications to Yb3+-Mn2+ and Yb3+-Cr3+ Halide Clusters and Implications to the Light Up-Conversion (M Atanasov et al.)Is a Dihydrogen Bond a Unique Phenomenon? (S J Grabowski & J Leszczynski) Readership: Graduate students and researchers in computational chemistry. Keywords:Computational Chemistry;Quantum Chemistry;Molecular Dynamics;Coupled Clusters Methods;Hydrogen Bonding;Molecular ElectronicsKey Features:Provides timely overviews of new findings and applications in a rapidly changing fieldIncludes reviews from well-known experts in the field, as well as current research data from the authors' groupsReviews:"This book is also an excellent source of information not only for advanced specialists, but also for graduate as well as undergraduate students."Professor W A Sokalski Wroclaw University of Technology "The contents of the book is quite well-balanced; there is a good mix of both somewhat general topics and topics that are of wide current interest. It will be useful and interesting for chemists, physicists and materials scientists."Professor Kang Hway Chuan National University of Singapore ' This important book collects together state-of-the-art reviews of diverse topics covering almost all the major areas of modern quantum chemistry. The current focus in the discipline of chemistry — synthesis, structure, reactivity and dynamics — is mainly on control. A variety of essential computational tools at the disposal of chemists have emerged from recent studies in quantum chemistry. The acceptance and application of these tools in the interfacial disciplines of the life and physical sciences continue to grow. The new era of modern quantum chemistry throws up promising potentialities for further research.Reviews of Modern Quantum Chemistry is a joint endeavor, in which renowned scientists from leading universities and research laboratories spanning 22 countries present 59 in-depth reviews. Along with a personal introduction written by Professor Walter Kohn, Nobel laureate (Chemistry, 1998), the articles celebrate the scientific contributions of Professor Robert G Parr on the occasion of his 80th birthday.List of Contributors: W Kohn, M Levy, R Pariser, B R Judd, E Lo, B N Plakhutin, A Savin, P Politzer, P Lane, J S Murray, A J Thakkar, S R Gadre, R F Nalewajski, K Jug, M Randic, G Del Re, U Kaldor, E Eliav, A Landau, M Ehara, M Ishida, K Toyota, H Nakatsuji, G Maroulis, A M Mebel, S Mahapatra, R Carbó-Dorca, Á Nagy, I A Howard, N H March, S-B Liu, R G Pearson, N Watanabe, S Ten-no, S Iwata, Y Udagawa, E Valderrama, X Fradera, I Silanes, J M Ugalde, R J Boyd, E V Ludeña, V V Karasiev, L Massa, T Tsuneda, K Hirao, J-M Tao, J P Perdew, O V Gritsenko, M Grüning, E J Baerends, F Aparicio, J Garza, A Cedillo, M Galván, R Vargas, E Engel, A Höck, R N Schmid, R M Dreizler, J Poater, M Solà, M Duran, J Robles, X Fradera, P K Chattaraj, A Poddar, B Maiti, A Cedillo, S Gutiérrez-Oliva, P Jaque, A Toro-Labbé, H Chermette, P Boulet, S Portmann, P Fuentealba, R Contreras, P Geerlings, F De Proft, R Balawender, D P Chong, A Vela, G Merino, F Kootstra, P L de Boeij, R van Leeuwen, J G Snijders, N T Maitra, K Burke, H Appel, E K U Gross, M K Harbola, H F Hameka, C A Daul, I Ciofini, A Bencini, S K Ghosh, A Tachibana, J M Cabrera-Trujillo, F Tenorio, O Mayorga, M Cases, V Kumar, Y Kawazoe, A M Köster, P Calaminici, Z Gómez, U Reveles, J A Alonso, L M Molina, M J López, F Dugue, A Mañanes, C A Fahlstrom, J A Nichols, D A Dixon, P A Derosa, A G Zacarias, J M Seminario, D G Kanhere, A Vichare, S A Blundell, Z-Y Lu, H-Y Liu, M Elstner, W-T Yang, J Muñoz, X Fradera, M Orozco, F J Luque, P Tarakeshwar, H M Lee, K S Kim, M Valiev, E J Bylaska, A Gramada, J H Weare, J Brickmann, M Keil, T E Exner, M Hoffmann & J Rychlewski. For courses covering pharmacology, and/or preparing nursing students for the pharmacology components of the NCLEX-RN® examination. PEARSON REVIEWS & RATIONALES: PHARMACOLOGY WITH "NURSING REVIEWS & RATIONALES", 3/e provides a clear, concentrated, and up-to-date review of today's "need to know" knowledge for effective pharmacology. Developed and reviewed by a large team of nurse educators, it can be used by current nursing students as a study aid, for NCLEX-RN® exam preparation, or by practicing nurses seeking comprehensive yet concise review of this discipline. Fully reflective of the current (2010) NCLEX-RN® Test Plan, it begins by introducing basic pharmacological principles and safety issues. Next, it provides complete chapters on each of the following: anti-infectives; antineoplastics; blood modifiers; medications for the cardiac, endocrine, gastrointestinal, immune, integumentary, neurological, musculoskeletal, renal, respiratory, and reproductive systems; psychiatric medications; visual and auditory medications; and herbal agents. This text comes with a complete support package, including access to additional questions and the complete eText online, and a tear-out NursingNotes card for clinical reference and quick review. The newly updated Eighth Edition of the top-selling NCLEX-RN® review is available in PDA format for easy study on the go. This edition reflects the current NCLEX® test plan and contains more than 5,000 total test questions—including alternate-format questions—to help students practice taking the exam. Organized by practice area—childbearing family and neonate, child health, adult medical-surgical, and psychiatric-mental health—this PDA program contains more questions than any other NCLEX-RN® review, and explains the rationale for correct and incorrect answers. Five comprehensive tests resembling the format of the NCLEX-RN® are also included. Platform: Palm OS, Windows CE, and Pocket PC handheld devices Global attention in scientific, industrial, and governmental communities to traces of toxic chemicals in foodstuffs and in both abiotic and biotic environ ments has justified the present triumvirate of specialized publications in this field: comprehensive reviews, rapidly published progress reports, and archival documentations. These three publications are integrated and scheduled to pro vide in international communication the coherency essential for nonduplicative and current

progress in a field as dynamic and complex as environmental con tamination and toxicology. Until now there has been no journal or other publica tion series reserved exclusively for the diversified literature on "toxic" chemicals in our foods, our feeds, our geographical surroundings, our domestic animals, our wildlife, and ourselves. Around the world immense efforts and many talents have been mobilized to technical and other evaluations of natures, locales, magnitudes, fates, and toxicology of the persisting residues of these chemicals loosed upon the world. Among the sequelae of this broad new emphasis has been an inescapable need for an articulated set of authoritative publications where one could expect to find the latest important world literature produced by this emerging area of science together with documentation of pertinent ancil lary legislation. 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. 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 This volume comprises six chapters which explore the development and applications of the methods of computational chemistry. The first chapter is on new developments in coupled-cluster (CC) theory. The homotopy method is used to obtain complete sets of solutions of nonlinear CC equations. The correspondence between multiple solutions to the CCSD, CCSDT, and full CI equations is established, and the applications of the new approach in modeling molecular systems are discussed. The second chapter reviews the computational theory for the time-dependent calculations of a solution to the Schrödinger equation for two electrons and focuses on the development of propagators to the solution. The next chapter features a discussion on a new self-consistent field for molecular interactions (SCF-MI) scheme for modifying Roothaan equations in order to avoid basis set superposition errors (BSSE). This method is especially suitable for computations of intermolecular interactions. Details of the theory, along with examples of applications to nucleic acid base pair complexes, are given. This chapter is well complemented by the following chapter, which reports the current status of computational studies of aromatic stacking and hydrogen bonding interactions among nucleic acid bases. The next chapter reveals the possibility of calculating the kinetics of chemical reactions in biological systems from the first principles. The last chapter reviews the results of rigorous ab initio studies of the series of derivatives of methane, silane, and germane. The presented molecular and vibrational parameters complement experimental data for these systems. In addition, the theoretical approach allows the prediction of the effects of halogeno-substitutions on their structures and properties. Contents:In Search of the Relationship between Multiple Solutions Characterizing Coupled-Cluster Theories (P Piecuch & K Kowalski)Computational Time-Dependent Two-Electron Theory and Long-Time Propagators (C A Weatherford)Self-Consistent Field Theory of Weakly Bonded Systems (E Gianinetti et al.)Aromatic DNA Base Stacking and H-Bonding (J Sponer et al.)Direct Ab Initio Dynamics Methodology for Modeling Kinetics of Biological Systems (T N Truong & D K Maity)Molecular Structure and Vibrational IR Spectra of Fluoro, Chloro and Bromosubstituted Methanes, Silanes and Germanes: An Ab Anitio Approach (J S Kwiatkowski & J Leszczynski) Readership: Graduate students and researchers in computational chemistry. Keywords:DNA;RNA;Base Stacking;Base Pairing;Ab Initio;Molecular Interactions;DFT;AMBER;Biomolecular Force Fields;Coupled ClustersReviews:“The breadth of subjects in this volume is such that almost everyone in the field of computational chemistry will find something of interest here … the reviews and articles that are included are all well-written and cover their subjects expertly and in great depth.”Journal of the American Chemical Society The contributions collected in this volume complement volume 1 of this series, disclosing results of current developments in methodologies and applications of computational chemistry methods. The covered topics include fundamentals and applications of propagator calculations, as well as recent developments in the computationally efficient and accurate SAC-CI method, which allows calculation of various electronic states at the same time. SAC-CI studies of excited states of large molecular systems like porphyrins are reviewed, and its application to investigations of surface phenomena is discussed. The book also features a review of recent work on quantum Monte Carlo simulations. Furthermore, the book discusses the application of computational methods to biomolecules and, in particular, the application of the DFT methods to prediction of molecular structures and the IR spectrum of the DNA bases, as well as currently developed force field parameters and their application in molecular dynamics calculations of biologically important molecules. Lastly, there is a review of a quantum chemistry course which prepares students at the Department of Chemistry of ETH Zurich to perform their own ab initio studies. Contents:The Electron Propagator Picture of Molecular Electronic Structure (J V Ortiz)SAC-CI Method: Theoretical Aspects and Some Recent Topics (H Nakatsuji)Quantum Monte Carlo and Electronic Structure (R N Barnett & W A Lester, Jr.)Molecular Structure and Infrared Spectra of the DNA Bases and Their Derivatives: Theory and Experiment (M J Nowak et al.)Derivation and Assessment of a New Set of Ab Initio Potentials and Its Application to Molecular Dynamics Simulations of Biological Molecules in Vacuo, in Crystal and in Aqueous Solution (M Aida)Practical Exercises in Ab Initio Quantum Chemistry — the World Wide Web as a Teaching Environment (H P Lüthi et al.) Readership: Computational and other chemists, and physicists. keywords: Containing 1000 board-style questions and answers with explanations, Anesthesiology Key Words and Questions for the Boards provides a high-yield, efficient review for residents preparing for board examinations and practitioners preparing for recertification. The Research Review for School Leaders, Volume III is specifically designed as a practical resource for school leaders whose schedules preclude opportunities to locate and review key research on every issue they must address. It places comprehensive, current, and accessible reviews of educational research at their fingertips, and is organized to make the research and practices it summarizes useful to them in their professional endeavors. This is the third volume of the Review. Although the title has changed, its purpose and substance is continuous with the work of the earlier volumes. The first Annual Review of Research for School Leaders (1996) summarized research on the status of public schooling, interdisciplinary curriculum, and educational applications of computers. The second volume (1998) addressed the topics of middle-level education, the extracurriculum, mathematics education reform, and drop outs. The present Volume III offers educational leaders reviews of research on five timely educational issues: * citizenship education; * multicultural education; * gifted and talented education; * classroom assessment; and * scheduling. A basic premise of this volume is that, to make sound decisions, professionals need to be up to date on current research related to the problems with which they grapple. A second premise is that research cannot simply be imposed in a formulaic way on a local setting; the nature of the particular problem to be solved will always bear upon the relevance of research to a specific context. Thus, this volume is envisioned as a helpful resource for school leaders as they engage in important discussions of the research with teachers, school board members, parents, and other interested parties as they collaboratively seek effective resolutions to local educational problems. “The Current is a rare creature: a gripping thriller and page-turner but also a masterwork of mood and language—a meditation on memory and time. You’ll want to go fast at the same time you’ll be compelled to savor each and every word.” —Ivy Pochoda, author of Wonder Valley Tim Johnston, whose breakout debut Descent was called “astonishing,” “dazzling,” and “unforgettable” by critics, returns with The Current, a tour de force about the indelible impact of a crime on the lives of innocent people. In the dead of winter, outside a small Minnesota town, state troopers pull two young women and their car from the icy Black Root River. One is found downriver, drowned, while the other is found at the scene—half frozen but alive. What happened was no accident, and news of the crime awakens the community’s memories of another young woman who lost her life in the same river ten years earlier, and whose killer may still live among them. Determined to find answers, the surviving young woman soon realizes that she’s connected to the earlier unsolved case by more than just a river, and the deeper she plunges into her own investigation, the closer she comes to dangerous truths, and to the violence that simmers just below the surface of her hometown. Grief, suspicion, the innocent and the guilty—all stir to life in this cold northern town where a young woman can come home, but still not be safe. Brilliantly plotted and unrelentingly propulsive, The Current is a beautifully realized story about the fragility of life, the power of the past, and the need, always, to fight back. Volume 3 of Computational Chemistry: Reviews of Current Trends adds well to the first two volumes of the series, presenting results of current developments in the methodologies and the applications of computational chemistry methods. The topics covered include fundamentals and applications of multireference Brillouin-Wigner coupled-cluster theory, as well as recent developments in quantum-chemical modeling of the interaction of solute and solvent.The book also features a review of recent developments and applications of the model-core-potential method. The application of computational methods to gas-phase chemical reactions is discussed. In particular, stratospheric bromine chemistry and its relationship to depletion of stratospheric ozone is examined by theoretical methods. Also, fundamental phenomena of bonding in gas-phase radical-sulfur compounds are presented.Finally, the book gives a review of a hot area — chemistry on the Internet. In addition to a survey of relevant chemistry Internet resources, an overview of the current state of Internet application is provided.