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Quantum mechanics is the laws of ...

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and the fundamentals of quantum field theory lay the foundations for advanced studies in solid-state physics, nuclear, and elementary particle physics. The authors earlier book, Quantum Mechanics, was praised for its unsurpassed clarity.

Advances in Quantum Chemistry

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Edition will discover new and revised material in all chapters, including new case studies and examples. There's also a new chapter dedicated to computational enzymology that demonstrates how principles of quantum mechanics applied to organic reactions can be extended to biological systems. Computational Organic Chemistry covers a broad range of problems and challenges in organic chemistry where computational chemistry has played a significant role in developing new theories or where it has provided additional evidence to support experimentally derived insights. Readers do not have to be experts in quantum mechanics. The first chapter of the book introduces all of the major theoretical concepts and definitions of quantum mechanics followed by a chapter dedicated to computed spectral properties and structure identification. Next, the book covers: Fundamentals of organic

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chemistry Pericyclic reactions Diradicals and carbenes Organic reactions of anions Solution-phase organic chemistry Organic reaction dynamics The final chapter offers new computational approaches to understand enzymes. The book features interviews with preeminent computational chemists, underscoring the role of collaboration in developing new science. Three of these interviews are new to this edition. Readers interested in exploring individual topics in greater depth should turn to the book's ancillary website www.comporgchem.com, which offers updates and supporting information. Plus, every cited article that is available in electronic form is listed with a link to the article.

Practical Aspects of Computational Chemistry II: An Overview of the Last Two Decades and Current Trends gathers the discussion of

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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

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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

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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.

Quantum Mechanics: Concepts and Applications provides a clear,

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balanced and modern introduction to the subject. Written with the student's background and ability in mind the book takes an innovative approach to quantum mechanics by combining the essential elements of the theory with the practical applications: it is therefore both a textbook and a problem solving book in one self-contained volume. Carefully structured, the book starts with the experimental basis of quantum mechanics and then discusses its mathematical tools. Subsequent chapters cover the formal foundations of the subject, the exact solutions of the Schrödinger equation for one and three dimensional potentials, time-independent and time-dependent approximation methods, and finally, the theory of scattering. The text is richly illustrated throughout with many worked examples and numerous problems with step-by-step solutions designed to help the reader master the machinery of

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quantum mechanics. The new edition has been completely updated and a solutions manual is available on request. Suitable for senior undergraduate courses and graduate courses.

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