A Chemists Guide To Valence Bond Theory

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Chemistry: Introduction to the Periodic TableA Chemists Guide To Valence

Sason S. Shaik, PhD, is a Professor and the Director of the Lise Meitner-Minerva Center for Computational Quantum Chemistry in the Hebrew University in Jerusalem.He has been a Fulbright Fellow (1974-1979) and became a Fellow of the AAAS in 2005. Among his awards are the Israel Chemical Society Medal for the Outstanding Young Chemist (1987), the Alexander von Humboldt Senior Award in 1996-1999 ...

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This reference on current VB theory and applications presents a practical system that can be applied to a variety of chemical problems in a uniform manner. After explaining basic VB theory, it discusses VB applications to bonding problems, aromaticity and antiaromaticity, the dioxygen molecule, polyradicals, excited states, organic reactions, inorganic/organometallic reactions, photochemical reactions, and catalytic reactions. With a guide for performing VB calculations, exercises and answers, and numerous solved problems, this is the premier reference for practitioners and upper-level students.

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Divided into five major parts, the two volumes of this ready reference cover the tailoring of theoretical methods for biochemical computations, as well as the many kinds of biomolecules, reaction and transition state elucidation, conformational flexibility determination, and drug design. Throughout, the chapters gradually build up from introductory level to comprehensive reviews of the latest research, and include all important compound classes, such as DNA, RNA, enzymes, vitamins, and heterocyclic compounds. The result is in-depth and vital knowledge for both readers already working in the field as well as those entering it. Includes contributions by Prof. Ada Yonath (Nobel Prize in Chemistry 2009) and Prof. Jerome Karle (Nobel Prize in Chemistry 1985).

As chemical bonds are not observable, there are various theories and models for their description. This book presents a selection of conceptually very different and historically competing views on chemical bonding analysis from quantum chemistry and quantum crystallography. It not only explains the principles and theories behind the methods, but also provides practical examples of how to derive bonding descriptors with modern software and of how to interpret them.

Chemical Modelling: Applications and Theory comprises critical literature reviews of molecular modelling, both theoretical and applied. Molecular modelling in this context refers to modelling the structure, properties and reactions of atoms, molecules & materials. Each chapter is compiled by experts in their fields and provides a selective review of recent literature. With chemical modelling covering such a wide range of subjects, this Specialist Periodical Report serves as the first port of call to any chemist, biochemist, materials scientist or molecular physicist needing to acquaint themselves of major developments in the area. Volume 5 covers literature published from June 2005 to May 2007.

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.

This book introduces in a non-traditional way the laws of physical chemistry and its history starting in the 16th century. It reveals to the reader how physical chemists try to understand chemical processes in terms of physical laws. Hydrogen is the main focus of the book as its simplicity makes the relevant laws of nature easy to explain and its role in energetics in the near future is clear. With the basics at hand, the importance of hydrogen as a raw material in the industry and as an energy carrier in the near future is made clear. Only simple chemical processes are discussed and very little mathematics is used. Both the pleasure and use of this field of research are revealed to the interested reader. The expected readership is made of high school students, non-chemistry major freshmen, and general audience with an interest in chemistry. The real aim of this book is to prompt the reader to wonder.

This handbook on group theory is geared toward chemists and experimental physicists who use spectroscopy and require knowledge of the electronic structures of the materials they investigate. Accessible to undergraduate students, it takes an elementary approach to many of the key concepts. Rather than the deductive method common to books on mathematics and theoretical physics, the present volume introduces fundamental concepts with simple examples, relating them to specific chemical and physical problems. The text is centered on detailed analysis of examples. Since neither chemists nor spectroscopists require theorem proofs, very few appear here. Instead, the focus remains on the principal conclusions, their meaning, and their use. In keeping with the text's practical bias, the main results of group theory are presented in all sections as procedures, making possible their systematic and step-by-step-application. Each chapter contains problems that develop practical skill and provide a valuable supplement to the text.

A unique overview of the different kinds of chemical bonds that can be found in the periodic table, from the main-group elements to transition elements, lanthanides and actinides. It takes into account the many developments that have taken place in the field over the past few decades due to the rapid advances in quantum chemical models and faster computers. This is the perfect complement to "Chemical Bonding - Fundamentals and Models" by the same editors, who are two of the top scientists working on this topic, each with extensive experience and important connections within the community.

In the 1970s, Density Functional Theory (DFT) was borrowed from physics and adapted to chemistry by a handful of visionaries. Now chemical DFT is a diverse and rapidly growing field, its progress fueled by numerous developing practical descriptors that make DFT as useful as it is vast. With 34 chapters written by 65 eminent scientists from 13 different countries, Chemical Reactivity Theory: A Density Functional View represents the true collaborative spirit and excitement of purpose engendered by the study and use of DFT. This work instructs readers on how concepts from DFT can be used to describe, understand, and predict chemical reactivity. Prior knowledge is not required as early chapters, written by the field's original pioneers, cover basic ground-state DFT and its extensions to time-dependent systems, excited states, and spin-polarized molecules. While the text is accessible to senior undergraduate or beginning graduate students, experienced researchers are certain to find interesting new insights in the perspectives presented by these seasoned experts. This remarkable one-of-a-kind resource— Provides authoritative accounts on aspects of the theory of chemical reactivity Describes various global reactivity descriptors, such as electronegativity, hardness, and electrophilicity Introduces and analyzes the usefulness of local reactivity descriptors such as Fukui, shape, and electron localization functions Offers an in-depth analysis of how chemical reactivity changes during different physicochemical processes or in the presence of external perturbations The book covers a gamut of related topics such as methods for determining atoms-in-molecules, population analysis, electrostatic potential, molecular quantum similarity, aromaticity, and biological activity. It also discusses the role of reactivity concepts in industrial and other practical applications. Whether you are searching for new products or new research projects, this is the ultimate guide for understanding chemical reactivity.