DESCRIPTION

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.

ABOUT THE AUTHOR

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, the 2001 Kolthoff Award, the 2001 Israel Chemical Society Prize, and the 2007 Schrödinger Medal of WATOC. His research interests are in the use of quantum chemistry to develop paradigms that can pattern data and lead to the generation and solution of new problems. From 1981-1992, the main focus of his research was on valence bond theory and its relationship to MO theory, and during that time, he developed a general model of reactivity based on a blend of VB and MO
elements. In 1994, he entered the field of oxidation and bond activation by metal oxo catalysts and enzymes, an area where he has contributed several seminal ideas (e.g., two-state reactivity) that led to resolution of major controversies and new predictions.

Philippe C. Hiberty is Director of Research at the Centre National de la Recherche Scientifique (CNRS) and a member of the Theoretical Chemistry Group in the Laboratoire de Chimie Physique at the University of Paris-Sud. He taught quantum chemistry for years at the Ecole Polytechique in Palaiseau. He received the Grand Prix Philippe A. Guye from the French Academy of Sciences in 2002. Under the supervision of Professor Lionel Salem, he devoted his PhD to building a bridge between MO and VB theories by devising a method for mapping MO wave functions to VB ones. In collaboration with Professor Sason Shaik, he applied VB theory to fundamental concepts of organic chemistry such as aromaticity, hypervalence, odd-electron bonds, prediction of reaction barriers from properties of reactants and products, and so on. He is the originator of the Breathing-Orbital Valence Bond method, which is aimed at combining the lucidity of compact VB wave functions with a good accuracy of the energetics.

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