Quantum Systems in Chemistry and Physics. Trends in Methods and Applications

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Book Condition: New. Publisher/Verlag: Springer Netherlands | Quantum Systems in Chemistry and Physics contains a refereed selection of the papers presented at the first European Workshop on this subject, held at San Miniato, near Pisa, Italy, in April 1996. The Workshop brought together leading experts in theoretical chemistry and molecular physics with an interest in the quantum mechanical many-body problem. This volume provides an insight into the latest research in this increasingly important field. Throughout the Workshop, the emphasis was on innovative theory and conceptual developments rather than on computational implementation. The various contributions presented reflect this emphasis and embrace topics such as density matrices and density functional theory, relativistic formulations, electron correlation, valence theory, nuclear motion, response theory, condensed matter, and chemical reactions. Audience: The volume will be of interest to those working in the molecular sciences and to theoretical chemists and molecular physicists in particular. | Preface. Introduction: The European Workshop `Quantum Systems in Chemistry and Physics; R. McWeeny. I: Trends in Methods. 1. Separability in Quantum Mechanics; R. McWeeny. 2. Optimized Effective Potential for Atoms and Molecules; T. Grabo, et al. 3. The Relativistic Quantum Defect Orbital Method and Some of Its Applications; I. Martin. 4. A...

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