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Quantum Theory for Chemical Applications Jochen Autschbach, 2020-12-07 Quantum theory and computational chemistry have become integral to the fields of chemistry chemical engineering and materials chemistry Concepts of chemical bonding band structure material properties and interactions between light and matter at the molecular scale tend to be expressed in the framework of orbital theory even when numerical calculations go beyond simple orbital models Yet the connections between these theoretical models and experimental observations are often unclear It is important now more than ever that students master quantum theory if they are going to apply chemical concepts In this book Jochen Autschbach connects the abstract with the concrete in an elegant way creating a guiding text for scholars and students alike *Quantum Theory for Chemical Applications* covers the quantum theory of atoms molecules and extended periodic systems Autschbach goes beyond standard textbooks by connecting the molecular and band structure perspectives covering response theory and more The book is broken into four parts Basic Theoretical Concepts Atomic Molecular and Crystal Orbitals Further Basic Concepts of Quantum Theory and Advanced Topics such as relativistic quantum chemistry and molecule light interactions The foresight Autschbach provides is immense and he sets up a solid theoretical background for nearly every quantum chemistry method used in contemporary research Because quantum theory tells us what the electrons do in atoms molecules and extended systems the pages in this book are full of answers to questions both long held and never before considered

Fundamentals of Quantum Mechanics James E. House, 2017-04-19 *Fundamentals of Quantum Mechanics* Third Edition is a clear and detailed introduction to quantum mechanics and its applications in chemistry and physics All required math is clearly explained including intermediate steps in derivations and concise review of the math is included in the text at appropriate points Most of the elementary quantum mechanical models including particles in boxes rigid rotor harmonic oscillator barrier penetration hydrogen atom are clearly and completely presented Applications of these models to selected real world topics are also included This new edition includes many new topics such as band theory and heat capacity of solids spectroscopy of molecules and complexes including applications to ligand field theory and small molecules of astrophysical interest Accessible style and colorful illustrations make the content appropriate for professional researchers and students alike Presents results of quantum mechanical calculations that can be performed with readily available software Provides exceptionally clear discussions of spin orbit coupling and group theory and comprehensive coverage of barrier penetration quantum mechanical tunneling that touches upon hot topics such as superconductivity and scanning tunneling microscopy Problems given at the end of each chapter help students to master concepts

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 Journal of the Society of Arts ,1860 *The Publishers Weekly* ,1917 **Fundamentals of Sustainable Chemical Science** Stanley E. Manahan,2009-03-10 Written by Stanley Manahan Fundamentals of Sustainable Chemical Science has been carefully designed to provide a basic introduction to chemistry including organic chemistry and biochemistry for readers with little or no prior background in the subject Manahan bestselling author of many environmental texts presents the material in a practical

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