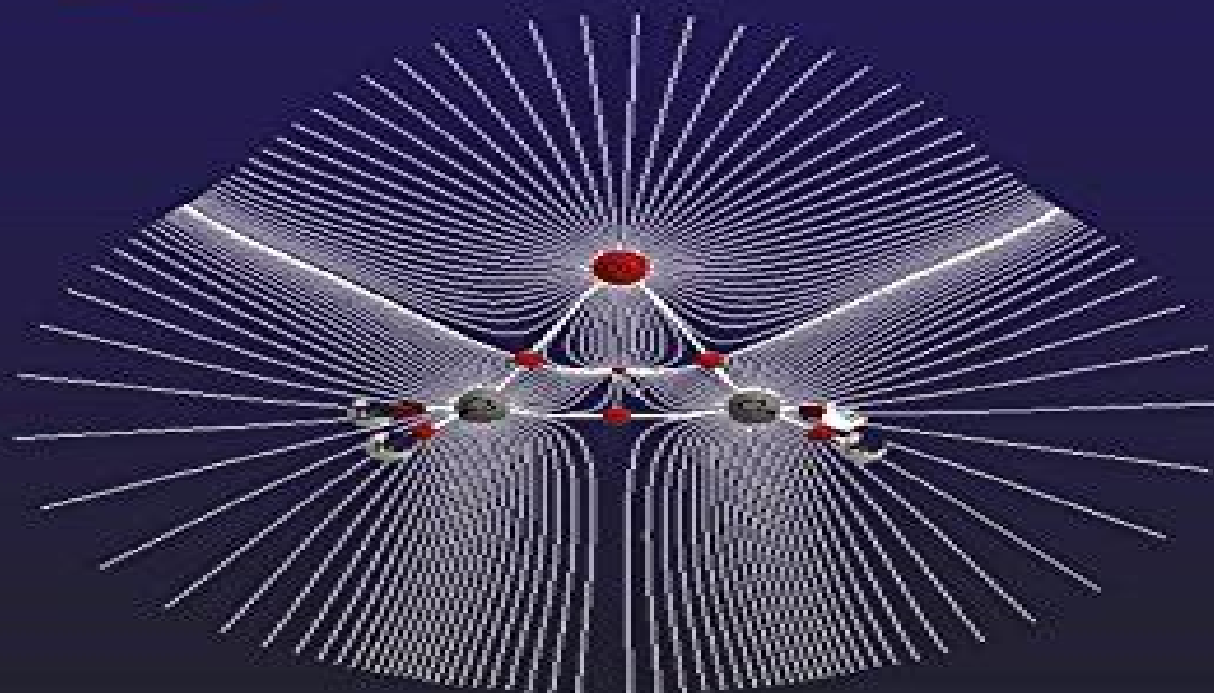


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Quantum Chemistry R.K. Prasad, 2006 The Third Edition Of Quantum Chemistry Is A Fully Updated Textbook Covering The Model Syllabus For M Sc General Course Recently Circulated By Ugc To All Indian Universities The Book Contains The Developments That Led To The Evolution Of Quantum Mechanics As Well As The Basic Concepts Of Quantum Mechanical Formalism In As Simple Terms As Possible The Exposition Of The Principles Is Followed By Application To Transnational Motion Of Micro Particles With Infinite And Finite Barriers Vibrational And Rotational Motions Perturbation And Variation Methods Atomic Structure Etc The Origins Of Chemical Bond Molecular Orbital And Valence Bond In Diatomic As Well As Polyatomic Molecules Are Elaborately Expanded With Sufficient Examples In Poly Electronic Atoms And Polyatomic Molecules The Apparently Complicated Theories Hfrscf Configuration Interaction Extended Huckel Theory Etc Are Presented With Utmost Clarity And Examples The Chapter On Molecular Symmetry And Group Theory Which Find Frequent Applications In Simplifying Problems Particularly In MO Treatment Is An Additional Feature Steps Involved In Mathematical Derivations Are Presented In Full Leaving No Ambiguity Illustrative Examples And Practice Problems With Hints Provided Are Given In Every Chapter The Book May Prove To Be A Self Educator

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Computational Chemistry: Introduction To The Theory And Applications Of Molecular And Quantum Mechanics Lewars, 2006-07-01

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addition to including the Hartree Fock method and post Hartree Fock methods *Quantum Chemistry of Solids* Robert A. Evarestov, 2013-01-19 *Quantum Chemistry of Solids* delivers a comprehensive account of the main features and possibilities of LCAO methods for the first principles calculations of electronic structure of periodic systems The first part describes the basic theory underlying the LCAO methods applied to periodic systems and the use of Hartree Fock HF Density Function theory DFT and hybrid Hamiltonians The translation and site symmetry consideration is included to establish connection between k space solid state physics and real space quantum chemistry The inclusion of electron correlation effects for periodic systems is considered on the basis of localized crystalline orbitals The possibilities of LCAO methods for chemical bonding analysis in periodic systems are discussed The second part deals with the applications of LCAO methods for calculations of bulk crystal properties including magnetic ordering and crystal structure optimization In the second edition two new chapters are added in the application part II of the book Chapter 12 deals with the recent LCAO calculations and illustrates the efficiency of the scalar relativistic LCAO method for solids containing heavy atoms Chapter 13 deals with the symmetry properties and the recent applications of LCAO method to inorganic nanotubes New material is added to chapter 9 devoted to LCAO calculations of perfect crystal properties The possibilities of LCAO method for calculation of the high frequency dielectric constants of crystals and the description of phase transitions in solids are discussed The efficiency of LCAO method in the quantum mechanics molecular dynamics approach to the interpretation of x ray absorption and EXAFS spectra is illustrated A new section is devoted to recent LCAO calculations of electronic vibrational and magnetic properties of tungstates MeWO₄ Me Fe Co Ni Cu Zn Cd

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