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Electronic Structure of MaterialsOrbital Approach to the Electronic Structure of SolidsElectronic Structure of Rare-Earth Nickelates from First-PrinciplesElectronic Structure and PropertiesElectronic Structure and Properties of Hydrogen in MetalsElectronic Structure of MaterialsElectronic Structure of AtomsThe electronic structure of molecules : a new approachElectronic Structure and the Properties of SolidsConnecting Electronic Structure with Inter-atomic PotentialsAdvanced Theories and Computational Approaches to the Electronic Structure of MoleculesThe Electronic Structure of AtomsPerspectives in Electronic Structure TheoryThe Electronic Structure of Complex SystemsElectronic Structure of MaterialsThe Electronic Structure of MoleculesMonte Carlo for the Electronic Structure in MoleculesAtomic and Electronic Structure of SurfacesElectronic Structure of Quantum Confined Atoms and MoleculesElectronic Structure of Molecules Rajendra Prasad Enric Canadell Harrison LaBollita Frank Y. Fradin C.B. Satterthwaite Adrian P. Sutton Amin Elsersawi John Wilfrid Linnett Walter A. Harrison Jessica L. McChesney C.E. Dykstra Roman F. Nalewajski P. Phariseau Mireille Defranceschi John W. Linnett Brian Lee Hammond Michel Lannoo K. D. Sen Linnett

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most textbooks in the field are either too advanced for students or don t adequately cover current research topics bridging this gap electronic structure of materials helps advanced undergraduate and graduate students understand electronic structure methods and enables them to use these techniques in their work developed from the author s lecture

this book provides an intuitive yet sound understanding of how structure and properties of solids may be related the natural link is provided by the band theory approach to the electronic structure of solids the chemically insightful concept of orbital interaction and the essential machinery of band theory are used throughout the book to build links between the crystal and electronic structure of periodic systems in such a way it is shown how important tools for understanding properties of solids like the density of states the fermi surface etc can be qualitatively sketched and used to either understand the results of quantitative calculations or to rationalize experimental observations extensive use of the orbital interaction approach appears to be a very efficient way of building bridges between physically and chemically based notions to understand the structure and properties of solids

this thesis demonstrates the value of theoretical approaches in the discovery of new superconducting materials it reports a detailed study of the recently discovered nickel oxide nickelate superconductors using multiple first principles computational tools from density functional theory to dynamical mean field theory in the context of superconductivity discoveries have generally been linked to serendipitous experimental discovery this thesis reports some of the few examples of predictions of new superconductors that have later been realized in practice a prime example of the significance of the methodology it expounds overall it represents a seminal systematic work in the electronic structure theory of the emergent field of nickelate superconductivity

treatise on materials science and technology volume 21 electronic structure and properties covers the developments in electron theory and electron spectroscopies the book discusses the electronic structure of perfect and defective solids the photoelectron spectroscopy as an electronic structure probe and the electron phonon interaction the text describes the elastic properties of transition metals the electrical resistivity of metals as well as the electronic structure of point defects in metals metallurgists materials scientists materials engineers and students involved in the related fields will find the book useful

hydrogen is the smallest impurity atom that can be implanted in a metallic host its small mass and strong interaction with the host electrons and nuclei are responsible for many anomalous and interesting solid state effects in addition hydrogen in metals gives rise to a number of technological problems such as hydrogen embrittlement hydrogen storage radiation hardening first wall problems associated with nuclear fusion reactors and degradation of the fuel cladding in fission reactors both the fundamental effects and applied problems have stimulated a great deal of inter est in the study of metal hydrogen systems in recent years this is evident from a growing list of publications as well as several international conferences held in this field during the past decade it is clear that a fundamental understanding of these problems re quires a firm knowledge of the basic interactions between hydrogen host metal atoms intrinsic lattice defects and electrons this understanding is made particularly difficult by hyrogen s small mass and by the large lattice distortions that accompany the hydrogenation process the purpose of the international symposium on the electronic structure and properties of hydrogen in metals held in richmond virginia march 4 6 1982 was to increase our fundamental under standing of hydrogen in

metals such knowledge is essential in solving technologically important questions the symposium con sisted of twenty two invited papers and seventy two contributed poster presentations and attracted nearly 150 participants from thirteen countries the proceedings of this symposium constitute this book

this book describes the modern real space approach to electronic structures and properties of crystalline and non crystalline materials in a form readily accessible to undergraduates in materials science physics and chemistry this book describes the modern real space approach to electronic structures and properties of crystalline and non crystalline materials in a form readily accessible to undergraduates in materials science physics and chemistry

the book presents the quantum theory of the electronic structure of atoms and focuses on the electronic structures and reactivity of atoms and molecules it shows how to draw molecules such as the oxygen and water to far more complex molecules using molecular orbital theory and hybridization of orbitals it gives quite clear picture of molecular polarity together with symmetrical and unsymmetrical distribution of an atom or molecule when developing a temporary instantaneous dipole the book provides a clear and comprehensive summary of oxidative and reductive processes electronegativity on oxidation and reduction is also introduced examples are provided it enables the reader to master the principles and applications of organic functional groups readers will find information quickly and easily about alkanes alkenes alkynes and arenes bonding with p and s is also introduced it explains the fundamental principles of nomenclature methods using iupac international union of pure and applied chemistry and enables the reader to apply it accurately and with confidence the book is replete with examples for guidance and there are extensive and complicated figures to direct the reader to nomenclature quickly it gives hands on chemistry activities with real life functions it provides clear and thorough understanding of carbohydrates polysaccharides starch and glycogen cellulose and chitin nucleotide nitrogenous hydroxyl and phosphate lipids protein ester lipoprotein glycolipid steroid mucin etc it is a useful reference for health professionals practicing physicists chemists and materials scientists

should be widely read by practicing physicists chemists and materials scientists philosophical magazine in this comprehensive and innovative text professor harrison stanford university offers a basic understanding of the electronic structure of covalent and ionic solids simple metals transition metals and their compounds the book illuminates the relationships of the electronic structures of these materials and shows how to calculate dielectric conducting and bonding properties for each also described are various methods of approximating electronic structure providing insight and even quantitative results from the comparisons dr harrison has also included an especially helpful solid state table of the elements that provides all the parameters needed to estimate almost any property of any solid with a hand held calculator using the techniques developed in the book designed for graduate or advanced undergraduate students who have completed an undergraduate course in quantum mechanics or atomic and modern physics the text treats the relation between structure and properties comprehensively for all solids rather than for small classes of solids this makes it an indispensable

reference for all who make use of approximative methods for electronic structure engineering semiconductor development and materials science the problems at the ends of the chapters are an important aspect of the book they clearly show that the calculations for systems and properties of genuine and current interest are actually quite elementary prefaces problems tables appendixes solid state table of the elements bibliography author and subject indexes will doubtless exert a lasting influence on the solid state physics literature physics today

that there have been remarkable advances in the field of molecular electronic structure during the last decade is clear not only to those working in the field but also to anyone else who has used quantum chemical results to guide their own investiga tions the progress in calculating the electronic structures of molecules has occurred through the truly ingenious theoretical and methodological developments that have made computationally tractable the underlying physics of electron distributions around a collection of nuclei at the same time there has been consider able benefit from the great advances in computer technology the growing sophistication declining costs and increasing accessibi lity of computers have let theorists apply their methods to prob lems in virtually all areas of molecular science consequently each year witnesses calculations on larger molecules than in the year before and calculations with greater accuracy and more com plete information on molecular properties we can surely anticipate continued methodological develop ments of real consequence and we can also see that the advance in computational capability is not about to slow down the recent introduction of array processors multiple processors and vector machines has yielded a tremendous acceleration of many types of computation including operations typically performed in quantum chemical studies utilizing such new computing power to the ut most has required some new ideas and some reformulations of existing methods

the understanding in science implies insights from several different points of view alternative modern outlooks on electronic structure of atoms and molecules all rooted in quantum mechanics are presented in a single text together these complementary perspectives provide a deeper understanding of the localization of electrons and bonds the origins of chemical interaction and reactivity behavior the interaction between the geometric and electronic structure of molecules etc in the opening two parts the basic principles and techniques of the contemporary computational and conceptual quantum chemistry are presented within both the wave function and electron density theories this background material is followed by a discussion of chemical concepts including stages of the bond formation processes chemical valence and bond multiplicity indices the hardness softness descriptors of molecules and reactants and general chemical reactivity stability principles the insights from information theory the basic elements of which are briefly introduced including the entropic origins and orbital communication theory of the chemical bond are the subject of part iv the importance of the non additive interference information tools in exploring patterns of chemical bonds and their covalent and ionic components will be emphasized

we present here the transcripts of lectures and talks which were delivered at the nato advanced study institute electronic structure of complex systems held at the state university of ghent belgium during the period july 12 23 1982 the aim of these lectures was to highlight some

of the current progress in our understanding of the electronic structure of com plex systems a massive leap forward is obtained in bandstructure calculations with the advent of linear methods the bandtheory also profitted tremendously from the recent developments in the density functional theories for the properties of the interacting electron gas in the presence of an external field of ions the means of per forming fast bandstructure calculations and the confidence in the underlying potential functions have led in the past five years or so to a wealth of investigations into the electronic properties of elemental solids and compounds the study of the trends of the electronic structure through families of materials provided invalu able insights for the prediction of new materials the detailed study of the electronic structure of specific solids was not neglected and our present knowledge of d and f metals and metal hydrides was reviewed for those systems we also investi gated the accuracy of the one electron potentials in fine detail and we complemented this with the study of small clusters of atoms where our calculations are amenable to comparison with the frontiers of quantum chemistry calculations

surfaces and interfaces play an increasingly important role in today s solid state devices in this book the reader is introduced in a didactic manner to the essential theoretical aspects of the atomic and electronic structure of surfaces and interfaces the book does not pretend to give a complete overview of contemporary problems and methods instead the authors strive to provide simple but qualitatively useful arguments that apply to a wide variety of cases the emphasis of the book is on semiconductor surfaces and interfaces but it also includes a thorough treatment of transition metals a general discussion of phonon dispersion curves and examples of large computational calculations the exercises accompanying every chapter will be of great benefit to the student

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