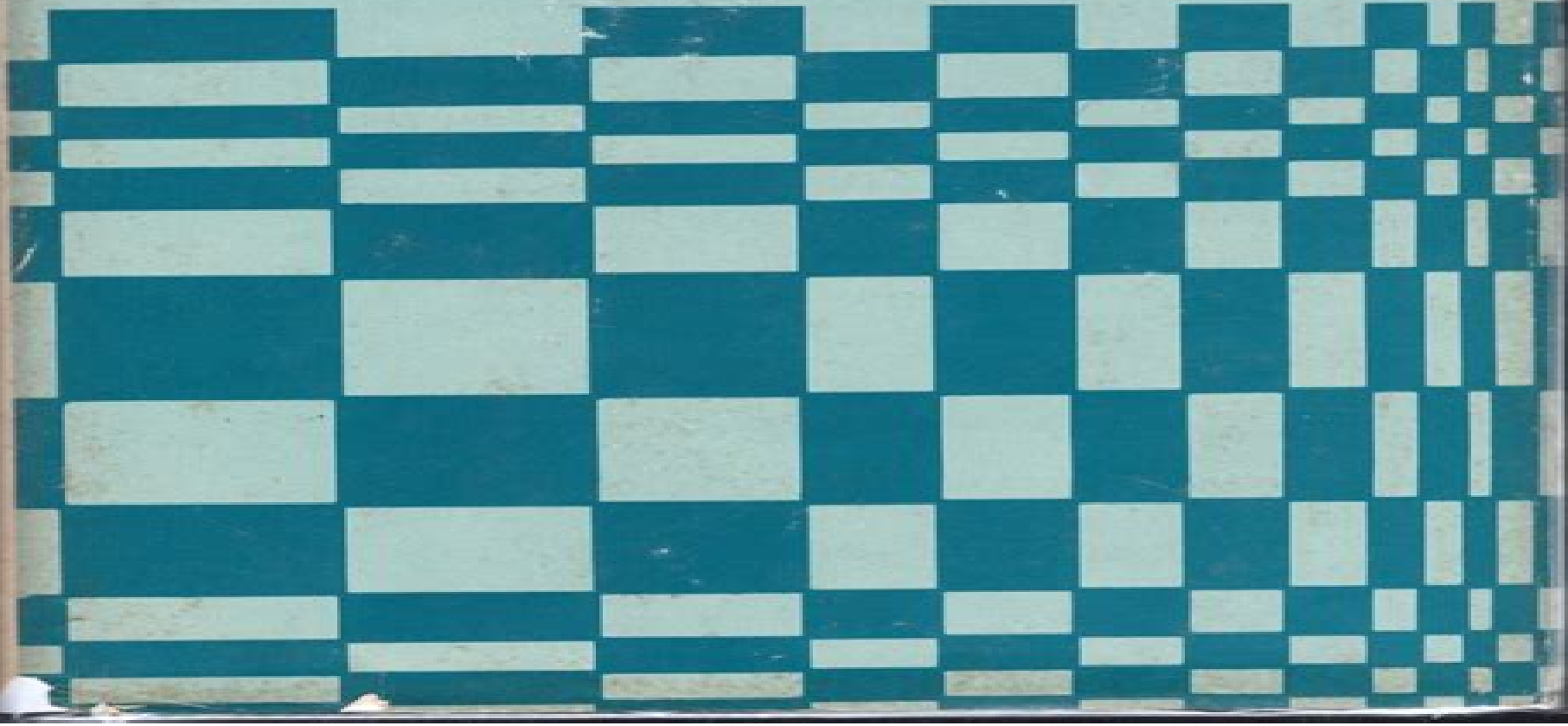
ELECTRONIC STRUCTURE IN SOLIDS

Edited by E. D. Haidemenakis



Electronic Structures In Solids

Hugues Dreysse

Electronic Structures In Solids:

Electronic Structure and the Properties of Solids Walter A. Harrison,2012-03-08 This text offers basic understanding of the electronic structure of covalent and ionic solids simple metals transition metals and their compounds also explains how to calculate dielectric conducting bonding properties **The Electronic Structures of Solids** B. R. Coles,A. D. Caplin,2013-10-22 The Electronic Structures of Solids aims to provide students of solid state physics with the essential concepts they will need in considering properties of solids that depend on their electronic structures and idea of the electronic character of particular materials and groups of materials The book first discusses the electronic structure of atoms including hydrogen atom and many electron atom The text also underscores bonding between atoms and electrons in metals Discussions focus on bonding energies and structures in the solid elements eigenstates of free electron gas and electrical conductivity The manuscript reviews the presence of electrons in metals as well as consequences of the periodic potential Brillouin zones and the nearly free electron model electronic structures of the metallic elements and calculation of band structures The text also ponders on metals insulators and semiconductors Topics include full and empty bands compound and doped semiconductors optical properties of solids and the dynamics of electron and holes The book is a dependable reference for readers and students of solid state physics interested in the electronic structure of solids **Electronic Structures in Solids** E. D. Haidemenakis,2013-11-11 Electronic Structure of Solids '91 Paul Ziesche,Helmut Eschrig,1991 *The Electronic Structure and Chemistry of Solids* P. A. Cox,2023 The Electronic Structure and Chemistry of Solids shows how the electronic structures and properties of solids can be described in terms familiar to chemists Recent years have seen a considerable growth of interest in chemical aspects of the electronic structure of solids The first three chapters give a fairly elementary account of the topics The later chapters present slightly more advanced aspects including many topics of current research interest such as metal insulator transitions low dimensional solids and molecular metals and the properties of surfaces The discussion is illustrated by a wide variety of examples **Orbital Approach to the Electronic Structure of Solids** Enric Canadell,Marie-Liesse Doublet,Christophe Iung,2012-01-12 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

Electronic Structures in Solids , *Orbital Approach to the Electronic Structure of Solids* Enric

Canadell,Marie-Liesse Doublet,Christophe Iung,2012-01-12 This book is aiming at filling the gap between the different languages of the physics and chemistry communities to understand the electronic structure of solids How structure and properties of solids are related is illustrated by considering in detail a large number of real examples *Electronic Structure and Magneto-Optical Properties of Solids* Victor Antonov,Bruce Harmon,Alexander Yaresko,2006-05-05 The aim of this book is to review recent achievements in thetheoretical investigations of the electronic structure optical magneto optical MO and x ray magnetic circular dichroism XMCD properties of compounds and Multilayered structures Chapter 1 of this book is of an introductory character and presentsthe theoretical foundations of the band theory of solids such as thedensity functional theory for ground state properties of solidsincluding local density approximation LDA It also presents somemodifications to the LDA such as gradient correction self interaction correction LDA U method orbital polarizationcorrection GW approximation and dynamical mean field theory Thedescription of the magneto optical effects and linear response theoryare also presented The book describes the MO properties for a number of 3d materials such as elemental ferromagnetic metals Fe Co and Ni andparamagnetic metals in external magnetic fields Pd and Pt someimportant 3d compounds such as XPt3 X V Cr Mn Fe and Co Heusleralloys chromium spinel chalcogenides MnB and strongly correlatedmagnetite Fe304 It also describes the recent achievements in both theexperimental and theoretical investigations of the electronicstructure optical and MO properties of transition metal multilayeredstructures MLS The book presents also the MO properties of f band ferromagneticmaterials Tm Nd Sm Ce and La monochalcogenides some important Y

Electronic Structure Calculations for Solids and Molecules Jorge Kohanoff,2006-06-29 Electronic structure problems are studied in condensed matter physics and theoretical chemistry to provide important insights into the properties of matter This 2006 graduate textbook describes the main theoretical approaches and computational techniques from the simplest approximations to the most sophisticated methods It starts with a detailed description of the various theoretical approaches to calculating the electronic structure of solids and molecules including density functional theory and chemical methods based on Hartree Fock theory The basic approximations are thoroughly discussed and an in depth overview of recent advances and alternative approaches in DFT is given The second part discusses the different practical methods used to solve the electronic structure problem computationally for both DFT and Hartree Fock approaches Adopting a unique and open approach this textbook is aimed at graduate students in physics and chemistry and is intended to improve communication between these communities It also serves as a reference for researchers entering the field Electronic Structure and Physical Properties of Solids Hugues Dreysse,2008-01-11 A very comprehensive book enabling the reader to understand the basic formalisms used in electronic structure determination and particularly the Muffin Tin Orbitals methods The latest developments are presented providing a very detailed description of the Full Potential schemes This book will provide a real state of the art since almost all of the contributions on formalism have not been and will not be published

elsewhere This book will become a standard reference volume Moreover applications in very active fields of today s research on magnetism are presented A wide spectrum of such questions is covered by this book For instance the paper on interlayer exchange coupling should become a classic since there has been fantastic experimental activity for 10 years and this can be considered to be the final theoretical answer to this question This work has never been presented in such a complete form

Electronic Structure Richard M. Martin,2004-04-08 An important graduate textbook in condensed matter physics by highly regarded physicist **Electronic Structure and Optical Properties of Semiconductors** Marvin L. Cohen,James R. Chelikowsky,2012-12-06 We began planning and writing this book in the late 1970s at the suggestion of Manuel Cardona and Helmut Lotsch We also received considerable en couragement and stimulation from colleagues Some said there was a need for instructional material in this area while others emphasized the utility of a research text We tried to strike a compromise The figures tables and references are included to enable researchers to obtain quickly essential information in this area of semiconductor research For instructors and stu dents we attempt to cover some basic ideas about electronic structure and semiconductor physics with applications to real rather than model solids We wish to thank our colleagues and collaborators whose research re sults and ideas are presented here Special thanks are due to Jim Phillips who influenced us both during our formative years and afterwards We are grateful to Sari Yamagishi for her patience and skill with the typing and production of the manuscript Finally we acknowledge the great patience of Helmut Lotsch and Manuel Cardona Berkeley CA M L Cohen Minneapolis MN J R Chelikowsky March 1988 VII Contents 1 Introduction 1 2 Theoretical Concepts and Methods 4 2 1 The One Electron Model and Band Structure 7 2 2 Properties of En k 11 3 Pseudopotentials 16 3 1 The Empirical Pseudopotential Method 20 3 2 Self Consistent and Ab Initio Pseudopotentials 25 4 Response Functions and Density of States 30 4 1 Charge Density and Bonding 38 The electronic structure and chemistry of solids Paul Anthony Cox,1987

Electronic Structure of Disordered Alloys, Surfaces and Interfaces Ilja Turek,Václav Drchal,Josef Kudrnovský,Mojmír Sob,Peter Weinberger,2013-11-27 At present there is an increasing interest in the prediction of properties of classical and new materials such as substitutional alloys their surfaces and metallic or semiconductor multilayers A detailed understanding based on a thus of the utmost importance for fu microscopic parameter free approach is ture developments in solid state physics and materials science The interrela tion between electronic and structural properties at surfaces plays a key role for a microscopic understanding of phenomena as diverse as catalysis corrosion chemisorption and crystal growth Remarkable progress has been made in the past 10 15 years in the understand ing of behavior of ideal crystals and their surfaces by relating their properties to the underlying electronic structure as determined from the first principles Similar studies of complex systems like imperfect surfaces interfaces and mul tilayered structures seem to be accessible by now Conventional band structure methods however are of limited use because they require an excessive number of atoms per elementary cell and are not able to account fully for e g substitu tional disorder and the true semiinfinite geometry of surfaces Such problems

can be solved more appropriately by Green function techniques and multiple scattering formalism Atomic and Electronic Structure of Solids Efthimios Kaxiras,2003 This text is a modern treatment of the theory of solids dealing with the physics of electron and phonon states in crystals and how they determine the structure and properties of solids There is also an extensive treatment of defects in solids A number of modern topics are also explored **Structure and Bonding in Crystalline Materials** Gregory S. Rohrer,2001-07-19 One of the motivating questions in materials research today is how can elements be combined to produce a solid with specified properties This book is intended to acquaint the reader with established principles of crystallography and cohesive forces that are needed to address the fundamental relationship between the composition structure and bonding Starting with an introduction to periodic trends the book discusses crystal structures and the various primary and secondary bonding types and finishes by describing a number of models for predicting phase stability and structure Containing a large number of worked examples exercises and detailed descriptions of numerous crystal structures this book is primarily intended as an advanced undergraduate or graduate level textbook for students of materials science It will also be useful to scientists and engineers who work with solid materials **Solid State Materials Chemistry** Patrick M. Woodward,Pavel Karen,John S. O. Evans,Thomas Vogt,2021-04-01 This comprehensive textbook provides a modern self contained treatment for upper undergraduate and graduate level students It emphasizes the links between structure defects bonding and properties throughout and provides an integrated treatment of a wide range of materials including crystalline amorphous organic and nano materials Boxes on synthesis methods characterization tools and technological applications distil specific examples and support student understanding of materials and their design The first six chapters cover the fundamentals of extended solids while later chapters explore a specific property or class of material building a coherent framework for students to master core concepts with confidence and for instructors to easily tailor the coverage to fit their own single semester course With mathematical details given only where they strengthen understanding 400 original figures and over 330 problems for hands on learning this accessible textbook is ideal for courses in chemistry and materials science **Electronic Structure of Organic Semiconductors** Luís Alcácer,2018-12-07 Written in the perspective of an experimental chemist this book puts together some fundamentals from chemistry solid state physics and quantum chemistry to help with understanding and predicting the electronic and optical properties of organic semiconductors both polymers and small molecules The text is intended to assist graduate students and researchers in the field of organic electronics to use theory to design more efficient materials for organic electronic devices such as organic solar cells light emitting diodes and field effect transistors After addressing some basic topics in solid state physics a comprehensive introduction to molecular orbitals and band theory leads to a description of computational methods based on Hartree Fock and density functional theory DFT for predicting geometry conformations frontier levels and energy band structures Topological defects and transport and optical properties are then addressed and one of the most commonly used

transparent conducting polymers PEDOT PSS is described in some detail as a case study *Electronic Structure of Alloys, Surfaces and Clusters* Abhijit Mookerjee,D.D. Sarma,2002-11-28 Understanding the electronic structure of solids is a basic part of theoretical investigation in physics Application of investigative techniques requires the solid under investigation to be periodic However this is not always the case This volume addresses three classes of non periodic solids currently undergoing the most study alloys sur

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