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Localized to Itinerant Electronic Transition in Perovskite Oxides - John B. Goodenough 2003-09-04 Interest in the transition metal oxides with perovskite related structures goes back to the 1950s when the sodium tungsten bronzes NaxWO3 were shown to be metallic [1], the system Lal_xSr~MnO3 was found to contain a ferromagnetic conductive phase [2], and La0.sSr0.sCoO3 was reported to be a ferromagnetic metal, but with a peculiar magnetization of 1.5 #a/Co atom [3]. Stoichiometric oxide perovskites have the generic formula AMO3 in which the A site is at the center of a simple cubic array of M sites; the oxide ions form (180 ° 4)) M O M bridges to give an MO3 array of corner shared MO6/2 octahedra and the

larger A cations have twelvefold oxygen coordination. Mismatch between the A O and M O equilibrium bond lengths introduces internal stresses. A compressive stress on the MO3 array is accommodated by a lowering of the M O M bond angle from 180 ° to (180 ° 4)); a tensile stress on the M O M bonds is accommodated by the formation of hexagonal polytypes [4].

**Understanding Materials Science** - Rolf E. Hummel 2004-08-03

This introduction to materials science for engineers examines not only the physical and engineering properties of materials, but also their history, uses, development, and some of the implications of resource depletion, materials substitutions, and so forth. Topics covered include: the stone, copper, bronze, and iron ages; physical properties of metals, ceramics, and plastics; electrical and magnetic properties of metals, semiconductors, and insulators; band structure of metals; metallurgy of iron. This new edition includes new developments in the last five years, updated graphs and other dated information and references.

Fundamentals of the Physics of Solids - Jenö Sólyom 2008-11-18

The reader is holding the second volume of a three-volume textbook on sol- state physics. This book is the outgrowth of the courses I have taught for many years at Eötvös University, Budapest, for undergraduate and graduate students under the titles Solid-State Physics and Modern Solid-State Physics. The main motivation for the publication of my lecture notes as a book was that none of the truly numerous textbooks covered all those areas that I felt should be included in a multi-semester course. Especially, if the course strives to present solid-state physics in a uni?ed structure, and aims at d- cussing not only classic chapters of the subject matter but also (in more or less detail) problems that are of great

interest for today's researcher as well. Besides, the book presents a much larger material than what can be covered in a two- or three-semester course. In the ?rst part of the ?rst volume the analysis of crystal symmetries and structure goes into details that certainly cannot be included in a usual course on solid-state physics. The same applies, among others, to the discussion of the methods used in the determination of band structure, the properties of Fermi liquids and non-Fermi liquids, and the theory of unconventional superconductors in the present and third volumes. These parts can be assigned as supplementary reading for interested students, or can be discussed in advanced courses.

*Operando Research in Heterogeneous Catalysis* - Joost Frenken 2016-12-26

This book is devoted to the emerging field of techniques for visualizing atomic-scale properties of active catalysts under actual working conditions, i.e. high gas pressures and high temperatures. It explains how to understand these observations in terms of the surface structures and dynamics and their detailed interplay with the gas phase. This provides an important new link between fundamental surface physics and chemistry, and applied catalysis. The book explains the motivation and the necessity of operando studies, and positions these with respect to the more traditional low-pressure investigations on the one hand and the reality of industrial catalysis on the other. The last decade has witnessed a rapid development of new experimental and theoretical tools for operando studies of heterogeneous catalysis. The book has a strong emphasis on the new techniques and illustrates how the challenges introduced by the harsh, operando conditions are faced for each of these new tools. Therefore, one can also read this book as a collection of recipes for the development of operando instruments. At present, the number of

scientific results obtained under operando conditions is still limited and mostly focused on a simple test reaction, the catalytic oxidation of CO. This reaction thus forms a natural binding element between the chapters, linking the demonstrations of new techniques, and also connecting the theoretical and experimental studies. Some first results on other reactions are also presented. If there is one thing that can be concluded already in this early stage, it is that the catalytic conditions themselves can have dramatic effects on the structure and composition of the surfaces of catalysts, which, in turn can greatly affect the mechanisms, the activity, and the selectivity of the chemical reactions that they catalyze.

**Electrons in Metals and Semiconductors** - R.G. Chambers 2012-12-06 Solid-state physics has for many years been one of the largest and most active areas of research in physics, and the physics of metals and semiconductors has in turn been one of the largest and most active areas in solid-state physics. Despite this, it is an area in which new and quite unexpected phenomena - such as the quantum Hall effect - are still being discovered, and in which many things are not yet fully understood. It forms an essential part of any undergraduate physics course. A number of textbooks on solid-state physics have appeared over the years and, because the subject has now grown so large, the books too have usually been large. By aiming at a more limited range of topics, I have tried in this book to cover them within a reasonably small compass. But I have also tried to avoid the phrase 'It can be shown that. . . ', as far as possible, and instead to explain to the reader just why things are the way they are; and sometimes this takes a little longer. I hope that some readers at least will find this approach helpful. 1 The free-electron model 1. 1 THE CLASSICAL DRUDE THEORY The characteristic properties of

metals and semiconductors are due to their conduction electrons: the electrons in the outermost atomic shells, which in the solid state are no longer bound to individual atoms, but are free to wander through the solid.

**International Books in Print, 1995** - Barbara Hopkinson 1995

**Positrons in Solids** - P. Hautojärvi 2012-12-06

In condensed matter initially fast positrons annihilate after having reached equi librium with the surroundings. The interaction of positrons with matter is governed by the laws of ordinary quantum mechanics. Field theory and antiparticle properties enter only in the annihilation process leading to the emergence of energetic photons. The monitoring of annihilation radiation by nuclear spectroscopic methods provides valuable information on the electron-positron system which can directly be related to the electronic structure of the medium. Since the positron is a positive electron its behavior in matter is especially interesting to solid-state and atomic physi cists. The small mass quarantees that the positron is really a quantum mechanical particle and completely different from any other particles and atoms. Positron physics started about 25 years ago but discoveries of new features in its interac tion with matter have maintained continuous interest and increasing activity in the field. Nowadays it is becoming part of the "stock-in-trade" of experimental physics.

*Atomic Scale Dynamics at Surfaces* - Giorgio Benedek 2019-01-14

Experimental advances in helium atom scattering spectroscopy over the last forty years have allowed the measurement of surface phonon dispersion curves of more than 200 different crystal surfaces and overlayers of insulators, semiconductors and metals. The first part of the book presents, at a tutorial level, the fundamental concepts and methods in

surface lattice dynamics, and the theory of atom-surface interaction and inelastic scattering in their various approximations, up to the recent electron-phonon theory of helium atom scattering from conducting surfaces. The second part of the book, after introducing the experimentalist to He-atom spectrometers and the rich phenomenology of helium atom scattering from corrugated surfaces, illustrates the most significant experimental results on the surface phonon dispersion curves of various classes of insulators, semiconductors, metals, layered crystals, topological insulators, complex surfaces, adsorbates, ultra-thin films and clusters. The great potential of helium atom scattering for the study of atomic scale diffusion, THz surface collective excitations, including acoustic surface plasmons, and the future prospects of helium atom scattering are presented in the concluding chapters. The book will be valuable reading for all researchers and graduate students interested in dynamical processes at surfaces.

**Phase Separation in Soft Matter Physics** - Pulat K. Khabibullaev 2003-04-11

This is the first monograph devoted to investigation of the most complex physical processes of soft systems, including a wide class of solutions. It blends modern theoretical understanding and experimental results, proposing new methods and models for the description of several soft systems.

*Qualitative Valence-Bond Descriptions of Electron-Rich Molecules: Pauling "3-Electron Bonds" and "Increased-Valence" Theory* - R. D. Harcourt 2012-12-06

This book provides qualitative molecular orbital and valence-bond descriptions of the electronic structures for electron-rich molecules, with strong emphasis given to the valence-bond approach. Electron-rich molecules form an extremely large class of molecules, and the results of quantum mechanical studies

from different laboratories indicate that qualitative valence-bond descriptions for many of these molecules are incomplete in so far as they usually omit "long-bond" Lewis structures from elementary descriptions of bonding. For example, the usual representation for the electronic structure of the ground-state for 03 involves resonance between the (+1 o and Until standard Lewis structures ~ ~ (-I . b:'" ~d· . . . . , recently, any contribution to resonance of the "long-bond" (or spin-paired o •• / •• ,. . has been largely ignored. diradica~ Lewis structure However, it :0 . 0. . e-. . . . . _____ " has now been calculated to be a very important structure. For the ground-states of numerous other systems, calculations also indicate that "long-bond" structures are more important than is usually supposed, and therefore they should frequently be included in qualitative valence-bond descriptions of electronic structure. The book describes how this may be done, and some of the resulting consequences for the interpretation of the electronic structure, bond properties and reactivities of various electron-rich molecules. When appropriate, molecular orbital and valence bond descriptions of bonding are compared, and relationships that exist between them are derived.

**Solid-State Physics** - James Patterson 2010-12-08

While the standard solid state topics are covered, the basic ones often have more detailed derivations than is customary (with an empasis on crystalline solids). Several recent topics are introduced, as are some subjects normally included only in condensed matter physics. Lattice vibrations, electrons, interactions, and spin effects (mostly in magnetism) are discussed the most comprehensively. Many problems are included whose level is from "fill in the steps" to long and challenging, and the text is equipped with references and several comments about experiments with figures and tables.

The Role of Metal Ions in Biology, Biochemistry and Medicine - Michael Moustakas 2021-09-06

Metal ions are fundamental elements for the maintenance of the lifespan of plants, animals and humans. Their substantial role in biological systems was recognized a long time ago. They are essential for the maintenance of life and their absence can cause growth disorders, severe malfunction, carcinogenesis or death. They are protagonists as macro- or microelements in several structural and functional roles, participating in many bio-chemical reactions, and arise in several forms. They participate in intra- and intercellular communications, in maintaining electrical charges and osmotic pressure, in photosynthesis and electron transfer processes, in the maintenance of pairing, stacking and the stability of nucleotide bases and also in the regulation of DNA transcription. They contribute to the proper functioning of nerve cells, muscle cells, the brain and the heart, the transport of oxygen and to many other biological processes up to the point that we cannot even imagine a life without metals. In this book, the papers published in the Special Issue "The Role of Metal Ions in Biology, Biochemistry and Medicine" are summarized, providing a picture of metal ion uses in biology, biochemistry and medicine, but also pointing out the toxicity impacts on plants, animals, humans and the environment.

**Physics Briefs** - 1994

*Chemistry of Precious Metals* - Simon Cotton 1997-06-30

Some 20 years ago, I was privileged to share in writing a book on the descriptive chemistry of the 4d, 5d, 4f and 5f metals that included these eight elements within its compass (S.A. Cotton and F.A. Hart, The Heavy Transition Elements, Macmillan, 1975). This volume shares the same aim of covering the descriptive chemistry of silver, gold and the six platinum metals in some

detail at a level suitable for advanced undergraduate and postgraduate study. It does not attempt to be a comprehensive treatise on the chemistry of these metals. It attempts to fill a slot between the general text and the in-depth review or monograph. The organometallic chemistry is confined to a-bonded com pounds in normal oxidation states; compounds with IT-bonding ligands are generally excluded. Their inclusion would have increased the length of the book considerably and, moreover, their recent chemistry has been extensively and expertly reviewed in the new Comprehensive Organometallic Chemistry, II, eds G. Wilkinson, F.G.A. Stone and E.W. Abel, Pergamon, Oxford, 1995.

*Part I: Physical Chemistry. Part II: Solid State Physics* - Arthur S. Wightman 2013-12-11

The fourth volume of the Collected Works is devoted to Wigners contribution to physical chemistry, statistical mechanics and solid-state physics. One corner stone was his introduction of what is now called the Wigner function, while his paper on adiabatic perturbations foreshadowed later work on Berry phases. Although few in number, Wigners articles on solid-state physics laid the foundations for the modern theory of the electronic structure of metals.

*Handbook of the Band Structure of Elemental Solids* - Dimitris A. Papaconstantopoulos 2014-11-10

This handbook presents electronic structure data and tabulations of Slater-Koster parameters for the whole periodic table. This second edition presents data sets for all elements up to Z = 112, Copernicium, whereas the first edition contained only 53 elements. In this new edition, results are given for the equation of state of the elements together with the parameters of a Birch fit, so that the reader can regenerate the results and derive additional information, such as Pressure-Volume relations and variation of Bulk Modulus with

Pressure. For each element, in addition to the equation of state, the energy bands, densities of states and a set of tight-binding parameters is provided. For a majority of elements, the tight-binding parameters are presented for both a two- and three-center approximation. For the hcp structure, new three-center tight-binding results are given. Other new material in this edition include: energy bands and densities of states of all rare-earth metals, a discussion of the McMillan-Gaspari-Gyorffy theories and a tabulation of the electron-ion interaction matrix elements. The evaluation of the Stoner criterion for ferromagnetism is examined and results are tabulated. This edition also contains two new appendices discussing the effects of spin-orbit interaction and a modified version of Harrison's tight-binding theory for metals which puts the theory on a quantitative basis.

Electron Correlations in Molecules and Solids - Peter Fulde 2012-12-06

This volume bridges the gap between quantum chemistry and solid-state theory. The text develops new concepts for treating many-body and correlation effects, and deals with applications of the theory to molecules, semiconductors, transition metals, heavy-fermion systems, and the new high-Tc superconducting materials.

**Books in Series, 1985-89** - 1989

*Fundamentals of Semiconductors* - Peter YU 2007-05-08

Excellent bridge between general solid-state physics textbook and research articles packed with providing detailed explanations of the electronic, vibrational, transport, and optical properties of semiconductors "The most striking feature of the book is its modern outlook ... provides a wonderful foundation. The most wonderful feature is its efficient style of exposition ... an excellent book." Physics Today "Presents the theoretical derivations carefully and in

detail and gives thorough discussions of the experimental results it presents. This makes it an excellent textbook both for learners and for more experienced researchers wishing to check facts. I have enjoyed reading it and strongly recommend it as a text for anyone working with semiconductors ... I know of no better text ... I am sure most semiconductor physicists will find this book useful and I recommend it to them." Contemporary Physics Offers much new material: an extensive appendix about the important and by now well-established, deep center known as the DX center, additional problems and the solutions to over fifty of the problems at the end of the various chapters.

*Handbook of Modern Sensors* - Jacob Fraden 2006-04-29

Seven years have passed since the publication of the previous edition of this book. During that time, sensor technologies have made a remarkable leap forward. The sensitivity of the sensors became higher, the dimensions became smaller, the sel- tivity became better, and the prices became lower. What have not changed are the fundamental principles of the sensor design. They are still governed by the laws of Nature. Arguably one of the greatest geniuses who ever lived, Leonardo Da Vinci, had his own peculiar way of praying. He was saying, “Oh Lord, thanks for Thou do not violate your own laws. ” It is comforting indeed that the laws of Nature do not change as time goes by; it is just our appreciation of them that is being re?ned. Thus, this new edition examines the same good old laws of Nature that are employed in the designs of various sensors. This has not changed much since the previous edition. Yet, the sections that describe the practical designs are revised substantially. Recent ideas and developments have been added, and less important and nonessential designs were dropped. Probably the most dramatic recent progress in the sensor technologies relates to wide use of MEMS and

MEOMS (micro-electro-mechanical systems and micro-electro-opto-mechanical systems). These are examined in this new edition with greater detail. This book is about devices commonly called sensors. The invention of a -croprocessor has brought highly sophisticated instruments into our everyday lives.

**Forthcoming Books** - Rose Arny 2004

*Catalog of Copyright Entries. Third Series* - Library of Congress. Copyright Office 1975

**Pure and Applied Science Books, 1876-1982** - 1982
Over 220,000 entries representing some 56,000 Library of Congress subject headings. Covers all disciplines of science and technology, e.g., engineering, agriculture, and domestic arts. Also contains at least 5000 titles published before 1876. Has many applications in libraries, information centers, and other organizations concerned with scientific and technological literature. Subject index contains main listing of entries. Each entry gives cataloging as prepared by the Library of Congress. Author/title indexes. -

**Nitride Semiconductors and Devices** - Hadis Morkoç 2013-03-08
This timely monograph addresses an important class of semiconductors and devices that constitute the underlying technology for blue lasers. It succinctly treats structural, electrical and optical properties of nitrides and the substrates on which they are deposited, band structures of nitrides, optical processes, deposition and fabrication technologies, light-emitting diodes, and lasers. It also includes many tables and figures detailing the properties and performance of nitride semiconductors and devices.

**Topology in Condensed Matter** - Michael I. Monastyrsky 2006-02-04
This book reports new results in condensed matter physics

for which topological methods and ideas are important. It considers, on the one hand, recently discovered systems such as carbon nanocrystals and, on the other hand, new topological methods used to describe more traditional systems such as the Fermi surfaces of normal metals, liquid crystals and quasicrystals. The authors of the book are renowned specialists in their fields and present the results of ongoing research, some of it obtained only very recently and not yet published in monograph form.

Condensed Matter Applications of AdS/CFT - Andrea Amoretti 2017-07-09

The book deals with applications of the AdS/CFT correspondence to strongly coupled condensed matter systems. In particular, it concerns with the study of thermo-electric transport properties of holographic models exhibiting momentum dissipation and their possible applications to the transport properties of strange metals. The present volume constitutes one of the few examples in the literature in which the topic is carefully reviewed both from the experimental and theoretical point of view, including not only holographic results but also standard condensed matter achievements developed in the past decades. This work might be extremely useful both for scientific and pedagogical purposes.

**Spin Electronics** - Michael Ziese 2007-06-30

For 50 years conventional electronics has ignored the electron spin. The manipulation and utilisation of the electron spin heralds an exciting and rapidly changing era in electronics, combining the disciplines of magnetism and traditional electronics. The first generation of "spintronic" devices (such as read heads based on giant magnetoresistance or non-volatile magnetic random access memories) have already gained dominant positions in the market place. This volume, the first of its kind on spin electronics describes all the

essential topics for new researchers entering the field. It covers magnetism and semiconductor basics, micromagnetism, experimental techniques, materials science, device fabrication and new developments in spin-dependent processes. At the end of most chapters are a number of exercises and worked problems to aid the reader in understanding this fascinating new field.

**Solid State Physics** - John J. Quinn 2009-09-18

Intended for a two semester advanced undergraduate or graduate course in Solid State Physics, this treatment offers modern coverage of the theory and related experiments, including the group theoretical approach to band structures, Moessbauer recoil free fraction, semi-classical electron theory, magnetoconductivity, electron self-energy and Landau theory of Fermi liquid, and both quantum and fractional quantum Hall effects. Integrated throughout are developments from the newest semiconductor devices, e.g. space charge layers, quantum wells and superlattices. The first half includes all material usually covered in the introductory course, but in greater depth than most introductory textbooks. The second half includes most of the important developments in solid-state researches of the past half century, addressing e.g. optical and electronic properties such as collective bulk and surface modes and spectral function of a quasiparticle, which is a basic concept for understanding LEED intensities, X ray fine structure spectroscopy and photoemission. So both the fundamental principles and most recent advances in solid state physics are explained in a class-tested tutorial style, with end-of-chapter exercises for review and reinforcement of key concepts and calculations.

Books in Print - 1983

Books in print is the major source of information on books currently published and in print in the United States. The database provides the record of

forthcoming books, books in-print, and books out-of-print.

***π-Electron Magnetism*** - Jaume Veciana 2003-09-04

Celebrating Volume 100: Thirty years ago Springer-Verlag together with a distinguished Board of Editors started the series Structure and Bonding. Initially the series was set up to publish reviews from different fields of modern inorganic chemistry, chemical physics and biochemistry, where the general subject of chemical bonding involves a metal and a small number of associated atoms. Three years ago the aims of the series was refined to span the entire periodic table and address structure and bonding issues wherever they may be relevant. Not only the traditional areas of chemical bonding will be dealt with but also nanostructres, molecular electronics, supramolecular structure, surfaces and clusters. With these aims in mind it is noteworthy that Volume 100 effectively reinforces and illustrates these ideals and is titled Pi-Electron Magnetism from Molecules to Magnetic Materials.

**Topological Insulators** - Shun-Qing Shen 2013-01-11

Topological insulators are insulating in the bulk, but process metallic states present around its boundary owing to the topological origin of the band structure. The metallic edge or surface states are immune to weak disorder or impurities, and robust against the deformation of the system geometry. This book, the first of its kind on topological insulators, presents a unified description of topological insulators from one to three dimensions based on the modified Dirac equation. A series of solutions of the bound states near the boundary are derived, and the existing conditions of these solutions are described. Topological invariants and their applications to a variety of systems from one-dimensional polyacetalene, to two-dimensional quantum spin Hall effect and p-wave superconductors, and three-dimensional topological

insulators and superconductors or superfluids are introduced, helping readers to better understand this fascinating new field. This book is intended for researchers and graduate students working in the field of topological insulators and related areas. Shun-Qing Shen is a Professor at the Department of Physics, the University of Hong Kong, China.

Weekly Record - 1980

**Nitride Semiconductors and Devices** - Hadis Morkoç 1999-09-28

This timely monograph addresses an important class of semiconductors and devices that constitute the underlying technology for blue lasers. It succinctly treats structural, electrical and optical properties of nitrides and the substrates on which they are deposited, band structures of nitrides, optical processes, deposition and fabrication technologies, light-emitting diodes, and lasers. It also includes many tables and figures detailing the properties and performance of nitride semiconductors and devices.

Quantum Physics of Semiconductor Materials and Devices - Debdeep Jena 2022-06-25

"Quantum Phenomena do not occur in a Hilbert space. They occur in a laboratory". - Asher Peres Semiconductor physics is a laboratory to learn and discover the concepts of quantum mechanics and thermodynamics, condensed matter physics, and materials science, and the payoffs are almost immediate in the form of useful semiconductor devices. Debdeep Jena has had the opportunity to work on both sides of the fence - on the fundamental materials science and quantum physics of semiconductors, and in their applications in semiconductor electronic and photonic devices. In Quantum Physics of Semiconductors and Nanostructures, Jena uses this experience to make each topic as tangible and accessible as possible to students at all levels. Consider the simplest physical processes that occur

in semiconductors: electron or hole transport in bands and over barriers, collision of electrons with the atoms in the crystal, or when electrons and holes annihilate each other to produce a photon. The correct explanation of these processes require a quantum mechanical treatment. Any shortcuts lead to misconceptions that can take years to dispel, and sometimes become roadblocks towards a deeper understanding and appreciation of the richness of the subject. A typical introductory course on semiconductor physics would then require prerequisites of quantum mechanics, statistical physics and thermodynamics, materials science, and electromagnetism. Rarely would a student have all this background when (s)he takes a course of this nature in most universities. Jena's work fills in these gaps and gives students the background and deeper understanding of the quantum physics of semiconductors and nanostructures.

**Quantum Solid-State Physics** - Serghey V. Vonsovsky 2012-05-05

This book treats the major problems of the quantum physics of solids, ranging from fundamental concepts to topical issues. Rather than use a deductive method of exposition, the authors consider and analyze simple empirically established properties of solids and employ more complicated models only as the need arises. Detailed treatment is given of classical problems such as chemical bonding in crystals, the one-dimensional Schrödinger equation with a periodic potential, the metal-insulator criterion, and the quantum theory of band electron motion in external fields. Consideration is also given to topical problems such as neutron scattering by the crystal lattice, plasma and Fermi liquid effects, the theory of disordered systems, and the polaron. The reader is expected to know only the fundamentals of quantum mechanics and statistical physics. Compared with the Russian edition (Nauka, Moscow 1983), the

book has been substantially revised and enlarged, new sections have been written and recent results have been incorporated.

Iron-Based Superconductivity - Peter D. Johnson 2015-01-06

This volume presents an in-depth review of experimental and theoretical studies on the newly discovered Fe-based superconductors. Following the Introduction, which places iron-based superconductors in the context of other unconventional superconductors, the book is divided into three sections covering sample growth, experimental characterization, and theoretical understanding. To understand the complex structure-property relationships of these materials, results from a wide range of experimental techniques and theoretical approaches are described that probe the electronic and magnetic properties and offer insight into either itinerant or localized electronic states. The extensive reference lists provide a bridge to further reading. Iron-Based Superconductivity is essential reading for advanced undergraduate and graduate students as well as researchers active in the fields of condensed matter physics and materials science in general, particularly those with an interest in correlated metals, frustrated spin systems, superconductivity, and competing orders.

**Metal-Ligand Interactions in Chemistry, Physics and Biology** - N. Russo 2000-01-31

Proceedings of the NATO Advanced Study Institute, held in Cetraro (CS) Italy, from 1-12 September 1998

**Spin Fluctuations in Itinerant Electron Magnetism** - Toru Moriya 2012-12-06

Ferromagnetism of metallic systems, especially those including transition metals, has been a controversial subject of modern science for a long time. This controversy sterns from the apparent dual character of the d-electrons responsible for magnetism in transition metals, i.e., they are itinerant elec

trons described by band theory in their ground state, while at finite tem peratures they show various properties that have long been attributed to a system consisting of local magnetic moments. The most familiar example of these properties is the Curie-Weiss law of magnetic susceptibility obeyed by almost all ferromagnets above their Curie temperatures. At first the problem seemed to be centered around whether the d-elec trons themselves are localized or itinerant. This question was settled in the 1950s and early 1960s by various experimental investigations, in particular by observations of d-electron Fermi surfaces in ferromagnetic transition metals. These observations are generally consistent with the results of band calculations. Theoretical investigations since then have concentrated on explaining this dual character of d-electron systems, taking account of the effects of electron-electron correlations in the itinerant electron model. The problem in physical terms is to study the spin density fluctuati·ons, which are ne glected in the mean-field or one-electron theory, and their influence on the physical properties.

First Principles Approaches to Spectroscopic Properties of Complex Materials - Cristiana Di Valentin 2014-09-26

The series Topics in Current Chemistry presents critical reviews of the present and future trends in modern chemical research. The scope of coverage is all areas of chemical science including the interfaces with related disciplines such as biology, medicine and materials science. The goal of each thematic volume is to give the non-specialist reader, whether in academia or industry, a comprehensive insight into an area where new research is emerging which is of interest to a larger scientific audience. Each review within the volume critically surveys one aspect of that topic and places it within the context of the volume as a whole. The most significant developments of the last 5 to

10 years are presented using selected examples to illustrate the principles discussed. The coverage is not intended to be an exhaustive summary of the field or include large quantities of data, but should rather be conceptual, concentrating on the methodological thinking that will allow the non-specialist reader to understand the information presented. Contributions also offer an outlook on potential future developments in the field. Review articles for the individual volumes are invited by the volume editors. Readership: research chemists at universities or in industry, graduate students.