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# ELECTRONIC STRUCTURE OF DISORDERED ALLOYS, SURFACES AND INTERFACES

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I. Turek, V. Drchal, J. Kudrnovský, M. Šob, P. Weinberger

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# Electronic Structure Of Disordered Alloys Surfaces And Interfaces

**Ilja Turek, Václav Drchal, Josef  
Kudrnovsky**



## **Electronic Structure Of Disordered Alloys Surfaces And Interfaces:**

Electronic Structure of Disordered Alloys, Surfaces and Interfaces Ilja Turek, 1997 An introduction to the study of basic electronic and magnetic properties of complex materials such as alloys their surfaces interfaces and extended defects Part I explores theoretical background with chapters on the linear muffin tin orbital method Green function method coherent potential approximation self consistency within atomic sphere approximation and relativistic theory Part II is devoted to applications including magnetic properties numerical implementation and interatomic interactions in alloys Of interest to researchers in solid state theory surface science and computational materials research Annotation copyrighted by Book News Inc Portland OR

*Electronic Structure of Disordered Alloys, Surfaces and Interfaces* Ilja Turek, Václav Drchal, Josef Kudrnovský, 2014-09-01

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

Electronic Structure and Physical Properties of Solids Hugues Dreyse, 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 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

**Multiple Scattering Theory for Spectroscopies** Didier Sébilleau, Keisuke Hatada, Hubert Ebert, 2018-04-05 This edited book based on material presented at the EU Spec Training School on Multiple Scattering Codes and the following MSNano Conference is divided into two distinct parts The first part subtitled basic knowledge provides the basics of the multiple scattering description in spectroscopies enabling readers to understand the physics behind the various multiple scattering codes available for modelling spectroscopies The second part extended knowledge presents state of the art short chapters on specific subjects associated with improving of the actual description of spectroscopies within the multiple scattering formalism such as inelastic processes or precise examples of modelling *Electron and Photon Impact Ionisation and Related Topics 2002* L.U Ancarani, 2003-05-01 *Electron and Photon Impact Ionisation and Related Topics 2002* provides an overview of recent international research in the field of ionization by electron and photon impact Emphasizing multi particle coincidence studies such as  $e 2e$   $e 3e$  ionization excitation and double photo ionization the book contains 18 contributions of recent experim *Properties of Complex Inorganic Solids 2* Annemarie Meike, 2000 The triennial International Alloy Conferences IACs aim at the identification and promotion of the common elements developed in the study either experimental phenomenological or theoretical and computational of materials properties across materials types from metals to minerals To accomplish this goal the IACs bring together scientists from a wide spectrum of materials science including experiment theory modeling and computation incorporating a broad range of materials properties The first IAC IAC 1 took place in Athens Greece June 16 21 1996 The present volume of proceedings contains the papers presented at IAC 2 that took place in Davos Switzerland August 8 13 1999 The topics in this book fall into several themes which suggest a number of different classification schemes We have chosen a scheme that classifies the papers in the volume into the categories Microstructural Properties Ordering Kinetics and Diffusion Magnetic Properties and Elastic Properties We have juxtaposed apparently disparate approaches to similar physical processes in the hope of revealing the dynamic character of the processes under consideration We hope this will invigorate new kinds of discussion and reveal challenges and new avenues to the description and prediction of properties of materials in the solid state and the conditions that produce them

*Handbook of Magnetic Material for Motor Drive Systems* Keisuke Fujisaki, 2025-09-05 This handbook which builds on the previously published book *Magnetic Material for Motor Drive Systems* focuses on how to use magnetic material for electrical motor drive systems especially electrical vehicles and power electronics The volume is aimed at researchers and engineers working towards the realization of more efficient and down sized motor drive systems by utilizing magnetic materials with complex properties based on the operation of motors and power electronics The magnetic materials and the motor drive system have mutual interactive characteristics due to electromagnetically coupling with the same current and voltage so it is

extremely important to have both viewpoints In this handbook for that purpose the fundamental concepts of electrical engineering and magnetic science and engineering are described in detail At the same time in order to develop new materials from the viewpoint of motor drive systems and to utilize the magnetic material this handbook widely discusses the multi scale analysis technology that traces back to the magnetic domain structure and first principles calculations the basics of current materials and new magnetic materials the fundamental magnetic measurement technology of magnetic material and the application of magnetic technology It is expected that the knowledge gained through this title will greatly contribute to the coming EV society      **Computational Quantum Physics and Chemistry of Nanomaterials** Mojmir Šob, 2021-04-01 This Special Issue of Nanomaterials collects a series of original research articles providing new insight into the application of computational quantum physics and chemistry in research on nanomaterials It illustrates the extension and diversity of the field and indicates some future directions It provides the reader with an overall view of the latest prospects in this fast evolving and cross disciplinary field      **Electronic Structure and Properties** Frank Y. Fradin, 2013-10-22 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      *Electron Scattering in Solid Matter* Jan Zablouil, Robert Hammerling, László Szunyogh, Peter Weinberger, 2005-12-12 Addressing graduate students and researchers this book gives a very detailed theoretical and computational description of multiple scattering in solid matter Particular emphasis is placed on solids with reduced dimensions on full potential approaches and on relativistic treatments For the first time approaches such as the screened Korringa Kohn Rostoker method are reviewed considering all formal steps such as single site scattering structure constants and screening transformations and also the numerical point of view Furthermore a very general approach is presented for solving the Poisson equation needed within density functional theory in order to achieve self consistency Special chapters are devoted to the Coherent Potential Approximation and to the Embedded Cluster Method used for example for describing nanostructured matter in real space In a final chapter physical properties related to the single particle Green's function such as magnetic anisotropies interlayer exchange coupling electric and magneto optical transport and spin waves serve to illustrate the usefulness of the methods described      **Advanced Magnetic Materials** Leszek Malkinski, 2012-05-24 This book reports on recent progress in emerging technologies modern characterization methods theory and applications of advanced magnetic materials It covers broad spectrum of topics technology and characterization of rapidly quenched nanowires for information technology fabrication and properties of hexagonal ferrite films for microwave communication

surface reconstruction of magnetite for spintronics synthesis of multiferroic composites for novel biomedical applications optimization of electroplated inductors for microelectronic devices theory of magnetism of Fe Al alloys and two advanced analytical approaches for modeling of magnetic materials using Everett integral and the inverse problem approach This book is addressed to a diverse group of readers with general background in physics or materials science but it can also benefit specialists in the field of magnetic materials

*Nanomagnetism*, 2006-03-27 Nanoscience is of central importance in the physical and biological sciences and is now pervasive in technology However nanomagnetism has a special role to play as magnetic properties depend uniquely on both dimensionality and lengthscales Nanomagnetism is already central to data storage sensor and device technologies but is increasingly being used in the life sciences and medicine This volume aims to introduce scientists computer scientists engineers and technologists from diverse fields to this fascinating and technologically important new branch of nanoscience The volume should appeal to both the interested general reader but also to the researcher wishing to obtain an overview of this fast moving field The contributions come from acknowledged leaders in the field who each give authoritative accounts of key fundamental aspects of nanomagnetism to which they have themselves made a major contribution After a brief introduction by the editors Wu first surveys the fundamental properties of magnetic nanostructures The interlayer exchange interactions within magnetic multilayer structures is next discussed by Stiles Camley then discusses the static dynamic and thermal properties of magnetic multilayers and nanostructures followed by an account of the phenomenon of exchange anisotropy by Berkowitz and Kodama This latter phenomenon is widely in current read head devices for example The transport properties of nanostructures also are spectacular and again underpin computer technology as we see from the discussion of giant magnetoresistance GMR and tunnelling magnetoresistance TMR presented by Fert and his colleagues Beyond GMR and TMR we look to the field of spintronics where new electronic devices are envisioned and for which quantum computing may depend as discussed in the chapter by Flatte and Jonker The volume concludes with discussion of the recently discovered phenomenon of current induced switching of magnetization by Edwards and Mathon Subject is in the forefront of nanoscience All Section authors are leading figures in this key field Presentations are accessible to non specialists with focus on underlying fundamentals

**Electron Correlations and Materials**

**Properties** A. Gonis, Nicholas Kioussis, Mikael Ciftan, 2012-12-06 Over the last thirty years or so the attempts to identify the electronic origins of materials properties have proceeded along two distinct and apparently divergent methodologies On the one hand so called single particle methods are based on the study of a single electron moving in an effective field formed by the other electrons and the nuclei in the system Band theory as this approach is referred to has had impressive successes in determining the equilibrium properties such as structural stability volume and charge densities of specific materials notably metals Today even coherent phase diagrams based on a single underlying lattice for binary metallic alloys can be studied with considerable accuracy In spite of its serious and well understood limitations regarding the handling of correlations band

theory has been embraced by the materials scientist Its single particle nature endows the method with an economy of concepts which leads to a clear identification of mechanisms driving physical behavior at the electronic level This perceived clarity often tends to override legitimate concerns regarding the validity of the method or its ability to correctly identify the mechanisms in the first place The alternative methodology pursued in the study of quantum systems consists of what can be referred to as conventional many body theory This methodology is based on attempts to study explicitly the effects of interparticle correlations using a number of different formal approaches including but not limited to perturbation methods Green function equation of motion methods configuration interactions quantum Monte Carlo and others

**Spin Current** Sadamichi Maekawa, Sergio O. Valenzuela, Eiji Saitoh, Takashi Kimura, 2017 In a new branch of physics and technology called spin electronics or spintronics the flow of electrical charge usual current as well as the flow of electron spin the so called spin current are manipulated and controlled together This book is intended to provide an introduction and guide to the new physics and applications of spin current

**Multiscale Materials Modelling** Z. X. Guo, 2007-05-31 Multiscale materials modelling offers an integrated approach to modelling material behaviour across a range of scales from the electronic atomic and microstructural up to the component level As a result it provides valuable new insights into complex structures and their properties opening the way to develop new multi functional materials together with improved process and product designs Multiscale materials modelling summarises some of the key techniques and their applications The various chapters cover the spectrum of scales in modelling methodologies including electronic structure calculations mesoscale and continuum modelling The book covers such themes as dislocation behaviour and plasticity as well as the modelling of structural materials such as metals polymers and ceramics With its distinguished editor and international team of contributors Multiscale materials modelling is a valuable reference for both the modelling community and those in industry wanting to know more about how multiscale materials modelling can help optimise product and process design Reviews the principles and applications of mult scale materials modelling Covers themes such as dislocation behaviour and plasticity and the modelling of structural materials Examines the spectrum of scales in modelling methodologies including electronic structure calculations mesoscale and continuum modelling

**Atomistic Simulation Of Quantum Transport In Nanoelectronic Devices (With Cd-rom)** Yu Zhu, Lei Liu, 2016-05-20 Computational nanoelectronics is an emerging multi disciplinary field covering condensed matter physics applied mathematics computer science and electronic engineering In recent decades a few state of the art software packages have been developed to carry out first principle atomistic device simulations Nevertheless those packages are either black boxes commercial codes or accessible only to very limited users private research codes The purpose of this book is to open one of the commercial black boxes and to demonstrate the complete procedure from theoretical derivation to numerical implementation all the way to device simulation Meanwhile the affiliated source code constitutes an open platform for new researchers This is the first book of its kind We hope the book will make a

modest contribution to the field of computational nanoelectronics      **Technical Reports Awareness Circular : TRAC.**  
,1988-03      Electronic Structure of Materials Rajendra Prasad,2013-07-23 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 notes this classroom tested book takes a microscopic view of materials as composed of interacting electrons and nuclei It explains all the properties of materials in terms of basic quantities of electrons and nuclei such as electronic charge mass and atomic number Based on quantum mechanics this first principles approach does not have any adjustable parameters The first half of the text presents the fundamentals and methods of electronic structure Using numerous examples the second half illustrates applications of the methods to various materials including crystalline solids disordered substitutional alloys amorphous solids nanoclusters nanowires graphene topological insulators battery materials spintronic materials and materials under extreme conditions Every chapter starts at a basic level and gradually moves to more complex topics preparing students for more advanced work in the field End of chapter exercises also help students get a sense of numbers and visualize the physical picture associated with the problem Students are encouraged to practice with the electronic structure calculations via user friendly software packages



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