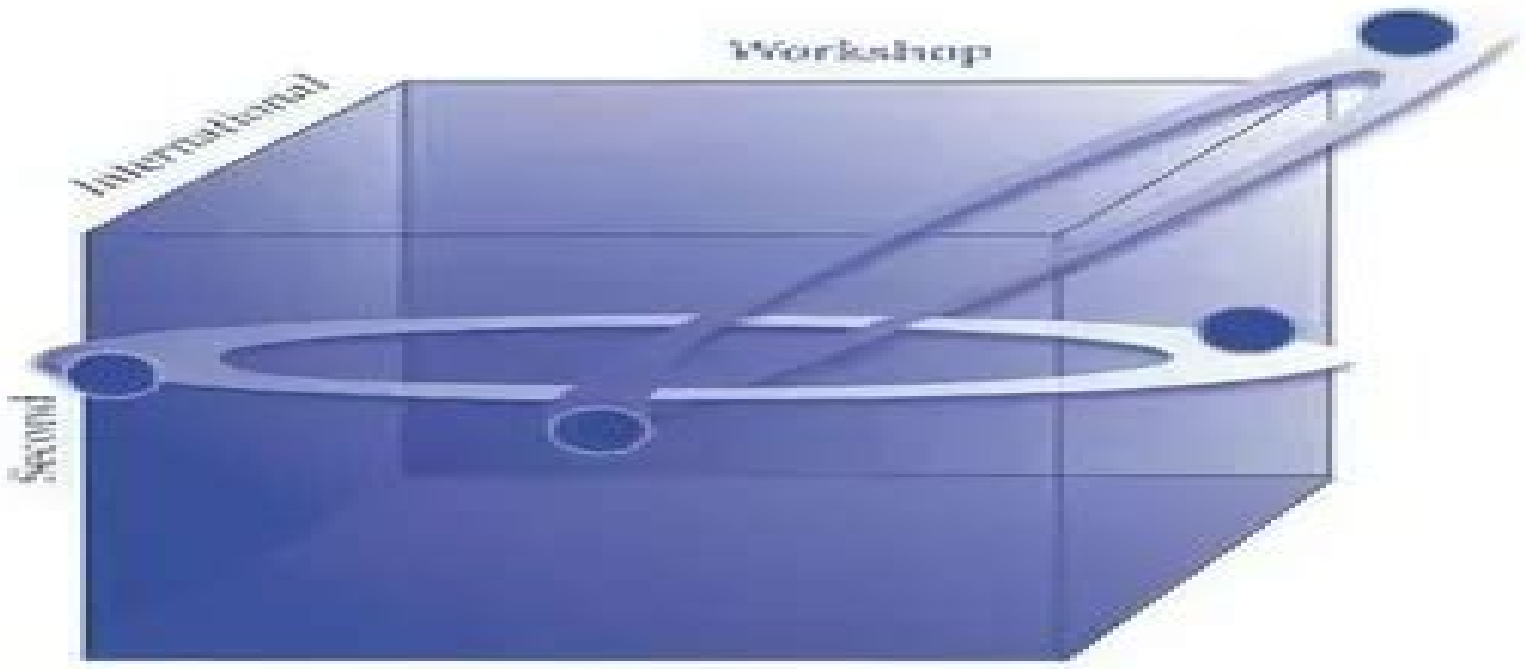
Electron Correlations and Materials Properties 2



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Electron Correlations And Materials Properties

Kurt Scharnberg,Sergei Kruchinin

Electron Correlations And Materials Properties:

Electron Correlations and Materials Properties A. Gonis,Nicholis 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 *Electron Correlations and Materials Properties* ,2006

Electron Correlations and Materials Properties 2 A. Gonis,Nicholis Kioussis,Mikael Ciftan,2014-01-15 **Electron Correlations and Materials Properties 2** A. Gonis,Nicholis Kioussis,Mikael Ciftan,2013-03-09 This is the second in a series of International Workshops on Electron Correlations and Materials Properties The aim of this series of workshops is to provide a periodic triennial and in depth assessment of advances in the study and understanding of the effects that electron electron interactions in solids have on the determination of measurable properties of materials The workshop is structured to include exposure to experimental work to phenomenology and to ab initio theory Since correlation effects are pervasive the workshop aims to concentrate on the identification of promising developing methodology experimental and theoretical addressing the most critical frontier issues of electron correlations on the properties of materials This series of workshops is distinguished from other topical meetings and conferences in that it strongly promotes an interdisciplinary approach to the study of correlations involving the fields of quantum chemistry physics and materials science The First Workshop was held June 28 July 3 1998 and a proceedings of the workshop was published by KluwerlPlenum The Second Workshop was held June 24 29 2001 and this volume contains the proceedings of that scientific meeting Through the publications of proceedings the workshop attempts to disseminate the information gathered during the discussions held at the Workshop to the wider scientific community and to establish a record of advances in the field **Special issue: Electron correlations and**

materials properties Antonios Gonis,Nick Kioussis,Peter Riseborough,2006 *Special Issue: Electron Correlations and Materials Properties* Antonios Gonis,2006 *Electron Correlation in New Materials and Nanosystems* Kurt Scharnberg,Sergei Kruchinin,2007-05-24 The articles collected in this book cover a wide range of materials with extraordinary superconducting and magnetic properties For many of the materials studied strong electronic correlations provide a link between these two phenomena which were long thought to be highly antagonistic The book reports both the progress in our understanding of fundamental physical processes and the advances made towards the development of devices Advances in Solid State Physics Bernhard Kramer,2003-09-22 Volume 43 of Advances in Solid State Physics contains the written versions of most of the plenary and invited lectures of the Spring Meeting of the Condensed Matter Physics section of the Deutsche Physikalische Gesellschaft held from March 24 to 28 2003 in Dresden Germany Many of the topical talks given at the numerous and very lively symposia are also included They covered an extremely interesting selection of timely subjects Thus the book truly reflects the status of the field of solid state physics in 2003 and explains its attractiveness not only in Germany but also internationally *Electronic Correlation Mapping* Jamal Berakdar,2008-07-11 An up to date selection of applications of correlation spectroscopy in particular as far as the mapping of properties of correlated many body systems is concerned The book starts with a qualitative analysis of the outcome of the two particle correlation spectroscopy of localized and delocalized electronic systems as they occur in atoms and solids The second chapter addresses how spin dependent interactions can be imaged by means of correlation spectroscopy both in spin polarized and extended systems A further chapter discusses possible pathways for the production of interacting two particle continuum states After presenting some established ways of quantifying electronic correlations and pointing out the relationship to correlation spectroscopy the author addresses in a separate chapter the electron electron interaction in extended systems and illustrates the ideas by some applications to fullerenes and metal clusters The last two chapters are devoted to the investigation of the potential of two particle spectroscopy in studying ordered surfaces and disordered samples Throughout the book the material is analyzed using rather qualitative arguments and the results of more sophisticated theories serve the purpose of endorsing the suggested physical scenarios The foundations of some of these theories have been presented in a corresponding volume entitled Concepts of Highly Excited Electronic Systems 3 527 40335 3 Electron Density Pratim Kumar Chattaraj,Debdutta Chakraborty,2024-07-10 Discover theoretical methodological and applied perspectives on electron density studies and density functional theory Electron density or the single particle density is a 3D function even for a many electron system Electron density contains all information regarding the ground state and also about some excited states of an atom or a molecule All the properties can be written as functionals of electron density and the energy attains its minimum value for the true density It has been used as the basis for a quantum chemical computational method called Density Functional Theory or DFT which can be used to determine various properties of molecules DFT brings out a drastic reduction

in computational cost due to its reduced dimensionality Thus DFT is considered to be the workhorse for modern computational chemistry physics as well as materials science Electron Density Concepts Computation and DFT Applications offers an introduction to the foundations and applications of electron density studies and analysis Beginning with an overview of major methodological and conceptual issues in electron density it analyzes DFT and its major successful applications The result is a state of the art reference for a vital tool in a range of experimental sciences Readers will also find A balance of fundamentals and applications to facilitate use by both theoretical and computational scientists Detailed discussion of topics including the Levy Perdew Sahni equation the Kohn Sham Inversion problem and more Analysis of DFT applications including the determination of structural magnetic and electronic properties Electron Density Concepts Computation and DFT Applications is ideal for academic researchers in quantum theoretical and computational chemistry and physics **A spin- and momentum-resolved photoemission study of strong electron correlation in Co/Cu(001)** Martin Ellguth,2015-06-15 Electron correlation is an important phenomenon of solid state physics which is actively studied both by experimentalists for the rich material properties which result from it and by theoreticians which face a lot of open questions on the way to a succesful many body description of electron systems where the Coulomb interaction plays an important role Ferromagnetic cobalt is an interesting candidate for the study of electron correlation since the exchange interaction splits the band structure into majority spin and minority spin bands which differ considerably in the strength of the electron electron interaction Using a revolutionary parallelized approach to spin resolved photoemission with an efficiency 3 to 4 orders of magnitude higher than previously possible the spin dependent manifestations of the electron correlation are revealed in unprecedented detail allowing for a characterization of the self energy As an additional phenomenon of the electron correlation unusual waterfall features previously only observed in superconductors occur in the photoemission spectra of cobalt Further subjects include a comprehensive mapping of the fcc cobalt Fermi surface and an investigation of unoccupied quantum well states in ultrathin cobalt films on copper accessed by spin resolved non linear photoemission The principle of the imaging spin filter and the data analysis routine are discussed in depth in a dedicated chapter

Magnetism And Electronic Correlations In Local-moment Systems: Rare-earth Elements And Compounds M Donath,Peter A Dowben,Wolfgang Nolting,1998-12-24 The interplay of magnetism and electronic correlations dominates the physical properties of many rare earth elements and their compounds The investigation of the mutual influence of the localized 4f electrons and itinerant band electrons represents a challenging task in theoretical as well as experimental physics Research areas of current interest are the electronic structure as determined from calculations and spectroscopies the magnetic properties in three and low dimensional systems open questions concerning transport such as spin disorder resistivity and the influence of structure and morphology *Properties and Applications of Thermoelectric Materials* Veljko Zlatic,Alexander Hewson,2009-06-24 As concerns with the efficient use of energy resources and the minimization of

environmental damage have come to the fore there has been a renewed interest in the role that thermoelectric devices could play in generating electricity from waste heat enabling cooling via refrigerators with no moving parts and many other more specialized applications The main problem in realizing this ambition is the rather low efficiency of such devices for general applications This book deals with the proceedings of a workshop addressed that problems by reviewing the latest experimental and theoretical work on suitable materials for device applications and by exploring various strategies that might increase their efficiency The proceedings cover a broad range of approaches from the experimental work of fabricating new compounds through to theoretical work in characterizing and understanding their properties The effects of strong electron correlation disorder the proximity to metal insulator transitions the properties of layered composite materials and the introduction of voids or cages into the structure to reduce the lattice thermal conductivity are all explored as ways of enhancing the efficiency of their use in thermoelectric devices Virtual Materials Design Norbert Huber,Surya R. Kalidindi,Stefan Blügel,Wolfgang Wenzel,2022-08-02 **Concepts in Electron Correlation** Alex C. Hewson,Veljko Zlatic,2012-12-06 The NATO sponsored Advanced Research Workshop on Concepts in Electron Correlation took place on the Croatian island of Hvar during the period from the 29th of September to the 3rd of October 2002 The topic of electron correlation is a fundamental one in the field of condensed matter and one that is being very actively studied both experimentally and theoretically at the present time The manifestations of electron cor relation are diverse and play an important role in systems ranging from high temperature superconductors heavy fermions manganite compounds with colossal magnetoresistance transition metal compounds with metal insulator transitions to mesoscopic systems and quantum dots The aim of the workshop was to provide an opportunity for a dialogue between exper imentalists and theoreticians to assess the current state of understanding and to set an agenda for future work There was also a follow up workshop on the same topic where the presentations included more background and introductory material for younger researchers in the field The papers presented in these proceedings clearly demonstrate the di versity of current research on electron correlation They show that real progress is being made in characterising systems experimentally and in developing theoretical approaches for a quantitative comparison with ex periment The more one learns however the more there is to understand and many of the contributions help to map out the territory which has yet to be explored We hope that the articles in this volume will be a stimulus for such future work Electronic Properties of Fullerenes Hans Kuzmany,Jörg Fink,Michael Mehring,Siegmar Roth,2012-12-06 Electronic Properties of Fullerenes and other Novel Materials gives an overview of the state of the art research It presents most recent results on preparation experimental analysis by electron spectroscopy infrared and Raman spectroscopy luminescence and nonlinear optical as well as possible technological applications Emphasis is also placed on the superconducting properties of Fullerenes The introductory and advanced contributions provide a good survey of the current status of this rapidly developing field **Electron Correlations in Molecules and Solids** Peter

Fulde,2012-12-06 Electron Correlations in Molecules and Solids bridges the gap between quantum chemistry and solid state theory In the first half of the text new concepts are developed for treating many body and correlation effects combining standard quantum chemical methods with projection techniques Greens function methods and Monte Carlo techniques The second half deals with applications of the theory to molecules semiconductors transition metals heavy fermion systems and the new high Tc superconducting materials **Quantum Simulations Of Condensed Matter Phenomena - International Workshop** James E Gubernatis,Jimmie D Doll,1989-12-01 The purpose of this workshop is to present and exchange information on rapidly growing areas in physics and chemistry where quantum simulation techniques are being developed and applied to the study of a variety of condensed matter phenomena These techniques include but are not limited to zero and finite temperature many electron Monte Carlo methods quantum spin systems techniques variational and Green s function Monte Carlo methods exact diagonalization studies of small clusters and studies of real time quantum dynamics by path integral and related approaches Physical Properties Of High Temperature Superconductors V Donald M Ginsberg,1996-04-20 The publication of Volume V of Physical Properties of High Temperature Superconductors is expected in March 1996 It will have chapters of interest for both fundamental studies and applied research The topics discussed are expected to include the electromagnetic response penetration depth and surface resistance local lattice distortions the influence of vortex fluctuations on macroscopic behavior the properties of superlattices and the symmetry of the superconducting order parameter **Optical Properties Of Low-dimensional Materials** Yoshihiko Kanemitsu,Tetsuo Ogawa,1996-01-18 This book surveys recent experimental and theoretical studies on optical properties of low dimensional materials e g artificial crystals in zeolites C60 and its related compounds silicon nanostructures including porous Si II VI and III V semiconductor quantum structures and Pb based natural quantum well systems The eight excellent detailed review articles are written by authorities on each field in Japan All the materials introduced in this book yield new optical phenomena originating from their mesoscopic and low dimensional characters contributing to a new research field of condensed matter and optical physics

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Electron Correlations And Materials Properties Introduction

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