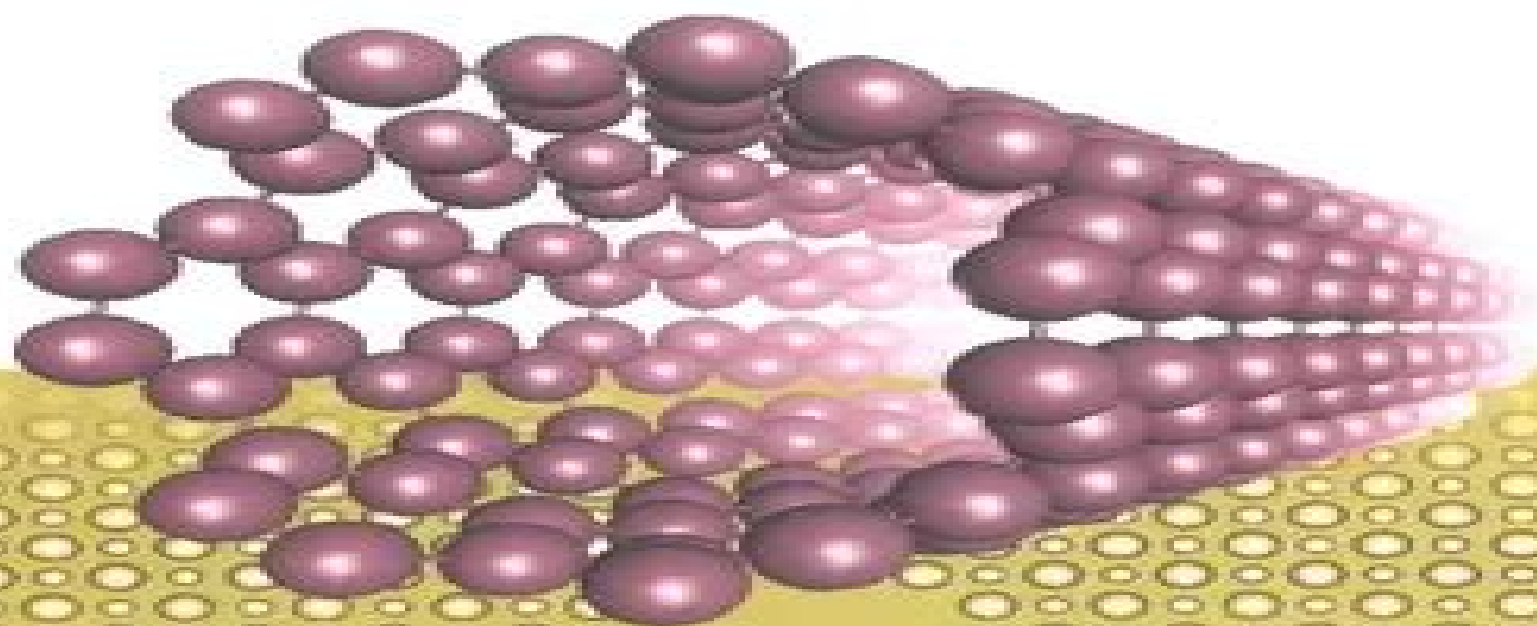


# First-Principles Calculations in Real-Space Formalism

Electronic Configurations and Transport  
Properties of Nanostructures



Kikuji Hirose • Tomoya Ono  
Yoshitaka Fujimoto • Shigeru Tsukamoto

Imperial College Press

# Firstprinciples Calculations In Realspace Formalism Electronic Configurations And Transport Properties Of Nanostructures

**Eckehard Schöll**



## **Firstprinciples Calculations In Realspace Formalism Electronic Configurations And Transport Properties Of Nanostructures:**

*First-principles Calculations In Real-space Formalism: Electronic Configurations And Transport Properties Of Nanostructures* Kikuji Hirose,Tomoya Ono,Yoshitaka Fujimoto,Shigeru Tsukamoto,2005-01-19 With cutting edge materials and minute electronic devices being produced by the latest nanoscale fabrication technology it is essential for scientists and engineers to rely on first principles ab initio calculation methods to fully understand the electronic configurations and transport properties of nanostructures It is now imperative to introduce practical and tractable calculation methods that accurately describe the physics in nanostructures suspended between electrodes This timely volume addresses novel methods for calculating electronic transport properties using real space formalisms free from geometrical restrictions The book comprises two parts The first details the basic formalism of the real space finite difference method and its applications This provides the theoretical foundation for the second part of the book which presents the methods for calculating the properties of electronic transport through nanostructures sandwiched by semi infinite electrodes a Electronic Structure Calculations on Graphics Processing Units Ross C. Walker,Andreas W. Goetz,2016-02-16 Electronic Structure Calculations on Graphics Processing Units From Quantum Chemistry to Condensed Matter Physics provides an overview of computing on graphics processing units GPUs a brief introduction to GPU programming and the latest examples of code developments and applications for the most widely used electronic structure methods The book covers all commonly used basis sets including localized Gaussian and Slater type basis functions plane waves wavelets and real space grid based approaches The chapters expose details on the calculation of two electron integrals exchange correlation quadrature Fock matrix formation solution of the self consistent field equations calculation of nuclear gradients to obtain forces and methods to treat excited states within DFT Other chapters focus on semiempirical and correlated wave function methods including density fitted second order Moller Plesset perturbation theory and both iterative and perturbative single and multireference coupled cluster methods Electronic Structure Calculations on Graphics Processing Units From Quantum Chemistry to Condensed Matter Physics presents an accessible overview of the field for graduate students and senior researchers of theoretical and computational chemistry condensed matter physics and materials science as well as software developers looking for an entry point into the realm of GPU and hybrid GPU CPU programming for electronic structure calculations *Topics In Nanoscience - Part Ii: Quantized Structures, Nanoelectronics, Thin Films Nanosystems: Typical Results And Future* Wolfram Schommers,2021-12-17 With the development of the scanning tunneling microscope nanoscience became an important discipline Single atoms could be manipulated in a controlled manner and it became possible to change matter at its ultimate level it is the level on which the properties of matter emerge This possibility enables to construct and to produce devices materials etc with very small sizes and completely new properties That opens up new perspectives for technology and is in

particular relevant in connection with nano engineering Nanosystems are unimaginably small and very fast No doubt this is an important characteristic But there is another feature possibly more relevant in connection with nanoscience and nanotechnology The essential point here is that we work at the ultimate level This is the smallest level at which the properties of our world emerge at which functional matter can exist In particular at this level biological individuality comes into existence This situation can be expressed in absolute terms This is not only the strongest material ever made this is the strongest material it will ever be possible to make D Ratner and M Ratner Nanotechnology and Homeland Security This is a very general statement All aspects of matter are concerned here Through the variation of the composition various forms of matter emerge with different items Nanosystems are usually small but they offer nevertheless the possibility to vary the structure of atomic molecular ensembles creating a diversity of new material specific properties A large variety of experimental possibilities come into play and flexible theoretical tools are needed at the basic level This is reflected in the different disciplines In nanoscience and nanotechnology we have various directions Materials science functional nanomaterials nanoparticles food chemistry medicine with brain research quantum and molecular computing bioinformatics magnetic nanostructures nano optics nano electronics etc The properties of matter which are involved within these nanodisciplines are ultimate in character i e their characteristic properties come into existence at this level The book is organized in this respect

**Sustainable Materials for Next Generation Energy Devices** Kuan Yew Cheong,Lung-Chien Chen,2020-12-01 Sustainable Materials for Next Generation Energy Devices Challenges and Opportunities presents the latest state of the art knowledge and innovation related to environmentally friendly functional materials that can be developed for and employed in producing a feasible next generation of energy storage and conversion devices The book is broken up into three sections covering Energy Storage Energy Conversion and Advanced Concepts It will be an important reference for researchers engineers and students who want to gain extensive knowledge in green and or sustainable functional materials and their applications Provides a concise resource for readers interested in sustainable and green functional materials for energy conversion and storage devices Emphasizes sustainable and green concepts in the design of energy devices based on renewable functional materials Presents a survey of both the challenges and opportunities available for renewable functional materials in the development of energy devices

**Nanoelectronic Materials** Loutfy H. Madkour,2019-06-27 This book presents synthesis techniques for the preparation of low dimensional nanomaterials including 0D quantum dots 1D nanowires nanotubes and 2D thin films few layers as well as their potential applications in nanoelectronic systems It focuses on the size effects involved in the transition from bulk materials to nanomaterials the electronic properties of nanoscale devices and different classes of nanomaterials from microelectronics to nanoelectronics to molecular electronics Furthermore it demonstrates the structural stability physical chemical magnetic optical electrical thermal electronic and mechanical properties of the nanomaterials Subsequent chapters address their characterization fabrication techniques from lab scale to

mass production and functionality In turn the book considers the environmental impact of nanotechnology and novel applications in the mechanical industries energy harvesting clean energy manufacturing materials electronics transistors health and medical therapy In closing it addresses the combination of biological systems with nanoelectronics and highlights examples of nanoelectronic cell interfaces and other advanced medical applications The book answers the following questions What is different at the nanoscale What is new about nanoscience What are nanomaterials NMs What are the fundamental issues in nanomaterials Where are nanomaterials found What nanomaterials exist in nature What is the importance of NMs in our lives Why so much interest in nanomaterials What is at nanoscale in nanomaterials What is graphene Are pure low dimensional systems interesting and worth pursuing Are nanotechnology products currently available What are sensors How can Artificial Intelligence AI and nanotechnology work together What are the recent advances in nanoelectronic materials What are the latest applications of NMs

**Handbook of Carbon Nanotubes** Jiji Abraham, Sabu Thomas, Nandakumar Kalarikkal, 2022-11-16 This Handbook covers the fundamentals of carbon nanotubes CNT their composites with different polymeric materials both natural and synthetic and their potential advanced applications Three different parts dedicated to each of these aspects are provided with chapters written by worldwide experts in the field It provides in depth information about this material serving as a reference book for a broad range of scientists industrial practitioners graduate and undergraduate students and other professionals in the fields of polymer science and engineering materials science surface science bioengineering and chemical engineering Part 1 comprises 22 chapters covering early stages of the development of CNT synthesis techniques growth mechanism the physics and chemistry of CNT various innovative characterization techniques the need of functionalization and different types of functionalization methods as well as the different properties of CNT A full chapter is devoted to theory and simulation aspects Moreover it pursues a significant amount of work on life cycle analysis of CNT and toxicity aspects Part 2 covers CNT based polymer nanocomposites in approximately 23 chapters It starts with a short introduction about polymer nanocomposites with special emphasis on CNT based polymer nanocomposites different manufacturing techniques as well as critical issues concerning CNT based polymer nanocomposites The text deeply reviews various classes of polymers like thermoset elastomer latex amorphous thermoplastic crystalline thermoplastic and polymer fibers used to prepare CNT based polymer composites It provides detailed awareness about the characterization of polymer composites The morphological rheological mechanical viscoelastic thermal electrical electromagnetic shielding properties are discussed in detail A chapter dedicated to the simulation and multiscale modelling of polymer nanocomposites is an additional attraction of this part of the Handbook Part 3 covers various potential applications of CNT in approximately 27 chapters It focuses on individual applications of CNT including mechanical applications energy conversion and storage applications fuel cells and water splitting solar cells and photovoltaics sensing applications nanofluidics nanoelectronics and microelectronic devices nano optics nanophotonics and nano optoelectronics

non linear optical applications piezo electric applications agriculture applications biomedical applications thermal materials environmental remediation applications anti microbial and antibacterial properties and other miscellaneous applications and multi functional applications of CNT based polymer nanocomposites One chapter is fully focussed on carbon nanotube research developments published papers and patents Risks associated with carbon nanotubes and competitive analysis of carbon nanotubes with other carbon allotropes are also addressed in this Handbook

**Advanced Nanoscale MOSFET Architectures** Kalyan Biswas, Angsuman Sarkar, 2024-06-12 Comprehensive reference on the fundamental principles and basic physics dictating metal oxide semiconductor field effect transistor MOSFET operation Advanced Nanoscale MOSFET Architectures provides an in depth review of modern metal oxide semiconductor field effect transistor MOSFET device technologies and advancements with information on their operation various architectures fabrication materials modeling and simulation methods circuit applications and other aspects related to nanoscale MOSFET technology The text begins with an introduction to the foundational technology before moving on to describe challenges associated with the scaling of nanoscale devices Other topics covered include device physics and operation strain engineering for highly scaled MOSFETs tunnel FET graphene based field effect transistors and more The text also compares silicon bulk and devices nanosheet transistors and introduces low power circuit design using advanced MOSFETs Additional topics covered include High k gate dielectrics and metal gate electrodes for multi gate MOSFETs covering gate stack processing and metal gate modification Strain engineering in 3D complementary metal oxide semiconductors CMOS and its scaling impact and strain engineering in silicon germanium SiGe FinFET and its challenges and future perspectives TCAD simulation of multi gate MOSFET covering model calibration and device performance for analog and RF applications Description of the design of an analog amplifier circuit using digital CMOS technology of SCL for ultra low power VLSI applications Advanced Nanoscale MOSFET Architectures helps readers understand device physics and design of new structures and material compositions making it an important resource for the researchers and professionals who are carrying out research in the field along with students in related programs of study

**Electronic Structure of Nanomaterials** Kristopher Edward Andersen, 2005 *Journal of the Physical Society of Japan*, 2016

**The British National Bibliography** Arthur James Wells, 2007 *Electronic Properties of Novel Nanostructures* Hans Kuzmany, 2005-10-20 All papers were peer reviewed The 19th Winterschool focused mainly on new nanostructured materials with data presented on functionalized fullerenes and carbon nanotubes filled and double wall nanotubes non carbon nanotubes such as BN and MoS<sub>2</sub> tubes and other nanostructures The direction of nanoelectronics research was explored in depth and advancements in composite technology and novel applications for nanotubes were discussed Importantly participants were updated on the theoretical and experimental determinations of structural and electronic properties as well as on characterization methods for molecular nanostructures

**Advanced Physics of Electron Transport in Semiconductors and Nanostructures** Massimo V. Fischetti, William G. Vandenberghe, 2016-05-20

This textbook is aimed at second year graduate students in Physics Electrical Engineering or Materials Science. It presents a rigorous introduction to electronic transport in solids especially at the nanometer scale. Understanding electronic transport in solids requires some basic knowledge of Hamiltonian Classical Mechanics Quantum Mechanics Condensed Matter Theory and Statistical Mechanics. Hence this book discusses those sub topics which are required to deal with electronic transport in a single self contained course. This will be useful for students who intend to work in academia or the nano micro electronics industry. Further topics covered include the theory of energy bands in crystals of second quantization and elementary excitations in solids of the dielectric properties of semiconductors with an emphasis on dielectric screening and coupled interfacial modes of electron scattering with phonons plasmons electrons and photons of the derivation of transport equations in semiconductors and semiconductor nanostructures somewhat at the quantum level but mainly at the semi classical level. The text presents examples relevant to current research thus not only about Si but also about III V compound semiconductors nanowires graphene and graphene nanoribbons. In particular the text gives major emphasis to plane wave methods applied to the electronic structure of solids both DFT and empirical pseudopotentials always paying attention to their effects on electronic transport and its numerical treatment. The core of the text is electronic transport with ample discussions of the transport equations derived both in the quantum picture the Liouville von Neumann equation and semi classically the Boltzmann transport equation BTE. An advanced chapter Chapter 18 is strictly related to the tricky transition from the time reversible Liouville von Neumann equation to the time irreversible Green's functions to the density matrix formalism and classically to the Boltzmann transport equation. Finally several methods for solving the BTE are also reviewed including the method of moments iterative methods direct matrix inversion Cellular Automata and Monte Carlo. Four appendices complete the text.

*First-principles Calculations and Model Hamiltonian Approaches to Electronic and Optical Properties of Defects, Interfaces and Nanostructures* Sangkook Choi, 2013. The dynamics of electrons governed by the Coulomb interaction determines a large portion of the observed phenomena of condensed matter. Thus the understanding of electronic structure has played a key role in predicting the electronic and optical properties of materials. In this dissertation I present some important applications of electronic structure theories for the theoretical calculation of these properties. In the first chapter I review the basics necessary for two complementary electronic structure theories model Hamiltonian approaches and first principles calculation. In the subsequent chapters I further discuss the applications of these approaches to nanostructures chapter II interfaces chapter III and defects chapter IV. The abstract of each section is as follows.

Section II 1 The sensitive structural dependence of the optical properties of single walled carbon nanotubes which are dominated by excitons and tunable by changing diameter and chirality makes them excellent candidates for optical devices. Because of strong many electron interaction effects the detailed dependence of the optical oscillator strength of excitons on nanotube diameter chiral angle and electronic subband index the so called family behavior however has been unclear. In this study

based on results from an extended Hubbard Hamiltonian with parameters derived from ab initio GW BSE calculations we have obtained an explicit formula for the family behavior of the oscillator strengths of excitons in semiconducting single walled carbon nanotubes SWCNTs incorporating environmental screening The formula explains well recent measurements and is expected to be useful in the understanding and design of possible SWCNT optical and optoelectronic devices

## Section II 2 Wave supercollimation in which a wavepacket is guided to move undistorted along a selected direction is a highly desirable property that is difficult to achieve for photons and has yet to be experimentally seen for electrons Disorder in a medium would inhibit supercollimation Here we report a counter intuitive phenomenon of electron supercollimation by disorder in graphene made possible by its Dirac fermion states We show that one can use one dimensional disorder potentials to control electron wavepacket transport along the potential fluctuation direction This is distinct from all known systems where the wavepacket would be further spread by the disorder and hindered in the potential fluctuating direction This phenomenon has significant implications in the understanding and applications of transport in graphene and other Dirac fermion materials

## Section III 1 The origin of magnetic flux noise in superconducting quantum interference devices with a power spectrum scaling as $1/f$ is frequency has been a puzzle for over 20 years This noise limits the decoherence time of superconducting qubits A consensus has emerged that the noise arises from fluctuating spins of localized electrons with an areal density of $5 \times 10^{17} \text{ m}^{-2}$ We show that the physical origin of the phenomenon are localized metal induced gap states at the interface In the presence of potential disorder at the metal insulator interface some of the metal induced gap states become localized and produce local moments A modest level of disorder yields the observed areal density

## Section III 2 We present a microscopic theory of disorder induced magnetic moment generation at nonmagnetic metal insulator interfaces Screened Hartree Fock solution of a tight binding Hamiltonian with electron electron interaction in which disorder is mimicked by the Anderson disorder model shows that magnetic moments are originated from localized metal induced gap states at the interface Magnetic moment areal density becomes saturated at a maximum value of $4 \times 10^{17} \text{ m}^{-2}$ as the disorder magnitude increases consistent with the observed universality of measured local magnetic moment areal density Dielectric screening effect is found to be essential for understanding the relatively universal behavior of the observed value

## Section IV 1 Optical initialization of the negatively charged nitrogen vacancy NV center in diamond makes it one of the best candidates for realization of addressable spins in the solid state for quantum computing and other studies However its exact mechanism was not clear We show that exact diagonalization of a many electron Hamiltonian with parameters derived from ab initio GW calculations puts strong constraints on the mechanism The energy surfaces of the low energy many body states and the relaxation processes of photo excitation responsible for the optical initialization are calculated Intersystem crossings are shown to be essential

## Section IV 2 Graphene has been predicted to be a good test material for atomic collapse theory due to its linear band structure with a Fermi velocity 300 times slower than the speed of light The Crommie group at UC Berkeley



measured using scanning tunneling microscopy electrons bound to the positively charged calcium dimers on graphene which corresponds to electrons collapsed to the super heavy nucleus in artificial atoms To compare measured bound states to atomic collapse theory in an artificial atom on graphene the net charges associated with calcium dimers should be quantified Here we quantified the net charges associated with a calcium dimer using density function theory

*Theory of Transport Properties of Semiconductor Nanostructures* Eckehard Schöll, 1997-12-31 Recent advances in the fabrication of semiconductors have created almost unlimited possibilities to design structures on a nanometre scale with extraordinary electronic and optoelectronic properties The theoretical understanding of electrical transport in such nanostructures is of utmost importance for future device applications This represents a challenging issue of today's basic research since it requires advanced theoretical techniques to cope with the quantum limit of charge transport ultrafast carrier dynamics and strongly nonlinear high field effects This book which appears in the electronic materials series presents an overview of the theoretical background and recent developments in the theory of electrical transport in semiconductor nanostructures It contains 11 chapters which are written by experts in their fields Starting with a tutorial introduction to the subject in Chapter 1 it proceeds to present different approaches to transport theory The semiclassical Boltzmann transport equation is in the centre of the next three chapters Hydrodynamic moment equations Chapter 2 Monte Carlo techniques Chapter 3 and the cellular automaton approach Chapter 4 are introduced and illustrated with applications to nanometre structures and device simulation A full quantum transport theory covering the Kubo formalism and nonequilibrium Green's functions Chapter 5 as well as the density matrix theory Chapter 6 is then presented

*Real-space Pseudopotential Calculations for the Electronic and Structural Properties of Nanostructures* Jiaxin Han, 2010 Nanostructures often possess unique properties which may lead to the development of new microelectronic and optoelectronic devices They also provide an opportunity to test fundamental quantum mechanical concepts such as the role of quantum confinement Considerable effort has been made to understand the electronic and structural properties of nanostructures but many fundamental issues remain In this work the electronic and structural properties of nanostructures are examined using several new computational methods The effect of dimensional confinement on quantum levels is investigated for hydrogenated Ge 110 using the plane wave density functional theory pseudopotential method We present a real space pseudopotential method for calculating the electronic structure of one dimensional periodic systems such as nanowires As an application of this method we examine H passivated Si nanowires The band structure and heat of formation of the Si nanowires are presented and compared to plane wave methods Our method is able to offer the same accuracy as the traditional plane wave methods but offers a number of computational advantages such as the ability to handle large systems and a better ease of implementation for highly parallel platforms Doping is important to many potential applications of nano regime semiconductors A series of first principles studies are conducted on the P doped Si 110 nanowires by the real space pseudopotential methods Nanowires of varied sizes

and different doping positions are investigated We calculate the binding energies of P atoms band gaps of the wires energetics of P atoms in different doping positions and core level shift of P atoms Defect wave functions of P atoms are also analyzed In addition we study the electronic properties of phosphorus doped silicon 111 nanofilms using the real space pseudopotential method Nanofilms with varied sizes and different doping positions are investigated We calculate the binding energies of P atoms band gaps of the films and energetics of P atoms in different doping positions Quantum confinement effects are compared with P doped Si nanocrystals and as well as nanowires We simulate the nanofilm STM images with P defects in varied film depths and make a comparison with the experimental measurement

*Calculations of Electronic Structures with Applications to Transport Properties and to Low Energy Electron Diffraction* Jesper Neve,1982 [Electronic Structure and Physical Properties of Solids](#) Hugues Dreyse,2014-01-15

**Electrical Transport in Nanoscale Systems** Massimiliano Di Ventra,2008-08-07 In recent years there has been a huge increase in the research and development of nanoscale science and technology Central to the understanding of the properties of nanoscale structures is the modeling of electronic conduction through these systems This graduate textbook provides an in depth description of the transport phenomena relevant to systems of nanoscale dimensions In this textbook the different theoretical approaches are critically discussed with emphasis on their basic assumptions and approximations The book also covers information content in the measurement of currents the role of initial conditions in establishing a steady state and the modern use of density functional theory Topics are introduced by simple physical arguments with particular attention to the non equilibrium statistical nature of electrical conduction and followed by a detailed formal derivation This textbook is ideal for graduate students in physics chemistry and electrical engineering

**Multiphysics in Nanostructures** Yoshitaka Umeno,Takahiro Shimada,Yusuke Kinoshita,Takayuki Kitamura,2017-07-13 This is the first book to systematically review and summarize the recent rapid advances and varied results of multiphysics in nanoscale materials including elastic strain engineering This book comprises topics on remarkable properties of multiphysics in low dimensional nanoscale components from first principles density functional theory or tight binding calculations which are essential for the nonlinear multiphysics couplings due to quantum mechanical effects This volume provides a clear point of view and insight into the varied work done in diverse fields and disciplines and promotes a fundamental to state of the art understanding of properties of multiphysics Because the novelty and complexity of mechanical and multiphysical properties of low dimensional nanostructures originate from combinations of outer shapes e g films wires tubes and dots and inner understructures e g grain boundaries domain walls vacancies and impurities the nanostructures are classified into fundamental elements and the properties of each element and their interplay are reviewed for systematic in depth understanding This book points out a new direction for multiphysics in nanostructures which opens the door both to exploiting and to designing novel functionalities at the nanoscale Readers will be interested in this rapidly expanding multidisciplinary work and will be motivated to enter this promising research area

*Electronic*

*Structure, Correlation Effects and Physical Properties of D- and F-metals and Their Compounds* Valentin Yu Irkhin, Yu. P. Irkhin, 2007 The book includes all main physical properties of d and f transition metal systems and corresponding theoretical concepts Special attention is paid to the theory of magnetism and transport phenomena Some examples of non traditional questions which are treated in detail in the book the influence of density of states singularities on electron properties many electron description of strong itinerant magnetism mechanisms of magnetic anisotropy microscopic theory of anomalous transport phenomena in ferromagnets Besides considering classical problems of solid state physics as applied to transition metals modern developments in the theory of correlation effects in d and f compounds are considered within many electron models The book contains where possible a simple physical discussion More difficult questions are considered in Appendices

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## **Firstprinciples Calculations In Realspace Formalism Electronic Configurations And Transport Properties Of Nanostructures Introduction**

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