

# Electronic Band Structure Calculation Nanohub Org Home

**Quantum Transport** Supriyo Datta.2005-06-16 This book presents the conceptual framework underlying the atomistic theory of matter, emphasizing those aspects that relate to current flow. This includes some of the most advanced concepts of non-equilibrium quantum statistical mechanics. No prior acquaintance with quantum mechanics is assumed. Chapter 1 provides a description of quantum transport in elementary terms accessible to a beginner. The book then works its way from hydrogen to nanostructures, with extensive coverage of current flow. The final chapter summarizes the equations for quantum transport with illustrative examples showing how conductors evolve from the atomic to the ohmic regime as they get larger. Many numerical examples are used to provide concrete illustrations and the corresponding Matlab codes can be downloaded from the web. Videostreamed lectures, keyed to specific sections of the book, are also available through the web. This book is primarily aimed at senior and graduate students.

**Cloud Computing and Software Services** Syed A. Ahson, Mohammad Ilyas.2010-07-19 Whether you're already in the cloud, or determining whether or not it makes sense for your organization, Cloud Computing and Software Services: Theory and Techniques provides the technical understanding needed to develop and maintain state-of-the-art cloud computing and software services. From basic concepts and recent research findings to fut

*Solar Cells and Modules* Arvind Shah.2020-07-16 This book gives a comprehensive introduction to the field of photovoltaic (PV) solar cells and modules. In thirteen chapters, it addresses a wide range of topics including the spectrum of light received by PV devices, the basic functioning of a solar cell, and the physical factors limiting the efficiency of solar cells. It places particular emphasis on crystalline silicon solar cells and modules, which constitute today more than 90 % of all modules sold worldwide. Describing in great detail both the manufacturing process and resulting module performance, the book also touches on the newest developments in this sector, such as Tunnel Oxide Passivated Contact (TOPCON) and heterojunction modules, while dedicating a major chapter to general questions of module design and fabrication. Overall, it presents the essential theoretical and practical concepts of PV solar cells and modules in an easy-to-understand manner and discusses current challenges facing the global research and development community.

**Making Grids Work** Marco Danelutto, Paraskevi Fragopoulou, Vladimir Getov.2010-11-04 Making Grids Work includes selected articles from the CoreGRID Workshop on Grid Programming Models, Grid and P2P Systems Architecture, Grid Systems, Tools and Environments held at the Institute of Computer Science, Foundation for Research and Technology - Hellas in Crete, Greece, June 2007. This workshop brought together representatives of the academic and industrial communities performing Grid research in Europe. Organized within the context of the CoreGRID Network of Excellence, this workshop provided a forum for the presentation and exchange of views on the latest developments in Grid Technology research. This volume is the 7th in the series of CoreGRID books. Making Grids Work is designed for a professional audience, composed of researchers and practitioners in industry. This volume is also suitable for graduate-level students in computer science.

**Electronic Energy Bands in Solids** L. Pincherle.1971

**Recent Advances in PMOS Negative Bias Temperature Instability** Souvik Mahapatra.2021-11-25 This book covers advances in Negative Bias Temperature Instability (NBTI) and will prove useful to researchers and professionals in the semiconductor devices areas. NBTI continues to remain

as an important reliability issue for CMOS transistors and circuits. Development of NBTI resilient technology relies on utilizing suitable stress conditions, artifact free measurements and accurate physics-based models for the reliable determination of degradation at end-of-life, as well as understanding the process, material and device architectural impacts. This book discusses: Ultra-fast measurements and modelling of parametric drift due to NBTI in different transistor architectures: planar bulk and FDSOI p-MOSFETs, p-FinFETs and GAA-SNS p-FETs, with Silicon and Silicon Germanium channels. BTI Analysis Tool (BAT), a comprehensive physics-based framework, to model the measured time kinetics of parametric drift during and after DC and AC stress, at different stress and recovery biases and temperature, as well as pulse duty cycle and frequency. The Reaction Diffusion (RD) model is used for generated interface traps, Transient Trap Occupancy Model (TTOM) for charge occupancy of the generated interface traps and their contribution, Activated Barrier Double Well Thermionic (ABDWT) model for hole trapping in pre-existing bulk gate insulator traps, and Reaction Diffusion Drift (RDD) model for bulk trap generation in the BAT framework; NBTI parametric drift is due to uncorrelated contributions from the trap generation (interface, bulk) and trapping processes. Analysis and modelling of Nitrogen incorporation into the gate insulator, Germanium incorporation into the channel, and mechanical stress effects due to changes in the transistor layout or device dimensions; similarities and differences of (100) surface dominated planar and GAA MOSFETs and (110) sidewall dominated FinFETs are analysed.

*Nanoscale Transistors* Mark Lundstrom, Jing Guo. 2006-06-18 To push MOSFETs to their scaling limits and to explore devices that may complement or even replace them at molecular scale, a clear understanding of device physics at nanometer scale is necessary. *Nanoscale Transistors* provides a description on the recent development of theory, modeling, and simulation of nanotransistors for electrical engineers, physicists, and chemists working on nanoscale devices. Simple physical pictures and semi-analytical models, which were validated by detailed numerical simulations, are provided for both evolutionary and revolutionary nanotransistors. After basic concepts are reviewed, the text summarizes the essentials of traditional semiconductor devices, digital circuits, and systems to supply a baseline against which new devices can be assessed. A nontraditional view of the MOSFET using concepts that are valid at nanoscale is developed and then applied to nanotube FET as an example of how to extend the concepts to revolutionary nanotransistors. This practical guide then explore the limits of devices by discussing conduction in single molecules

*An Electronic Band Structure Calculation of First Stage Potassium Graphite, KC8* David P. DiVincenzo. 1980-05-01 Master's Thesis, May, 1980

*Lessons from Nanoelectronics* Supriyo Datta. 2017 A. Basic concepts. Why electrons flow ; The elastic resistor ; Ballistic and diffusive transport ; Conductance from fluctuation ; Energy band model ; The nanotransistor ; Diffusion equation for ballistic transport ; Boltzmann equation ; Electrochemical potentials and quasi-Fermi levels ; Hall effect ; Smart contacts ; Thermoelectricity ; Phonon transport ; Second law ; Fuel value of information

**Computational Electronics** Dragica Vasileska, Stephen Goodnick. 2022-06-01 Computational Electronics is devoted to state of the art numerical techniques and physical models used in the simulation of semiconductor devices from a semi-classical perspective. Computational electronics, as a part of the general Technology Computer Aided Design (TCAD) field, has become increasingly important as the cost of semiconductor manufacturing has grown exponentially, with a concurrent need to reduce the time from design to manufacture. The motivation for this volume is the need within the modeling and simulation community for a comprehensive text which spans basic drift-diffusion modeling, through energy balance and hydrodynamic models, and finally particle based simulation. One unique feature of this book is a specific focus on numerical examples, particularly the use of commercially available software in the TCAD community. The concept for this book originated from a first year graduate course on computational electronics, taught now for several years, in the Electrical Engineering Department at Arizona State University. Numerous exercises and projects were derived from this course and have been included. The prerequisite knowledge is a fundamental understanding of basic

semiconductor physics, the physical models for various device technologies such as pn diodes, bipolar junction transistors, and field effect transistors. **Nanowire Field Effect Transistors: Principles and Applications** Dae Mann Kim, Yoon-Ha Jeong. 2013-10-23 "Nanowire Field Effect Transistor: Basic Principles and Applications" places an emphasis on the application aspects of nanowire field effect transistors (NWFET). Device physics and electronics are discussed in a compact manner, together with the p-n junction diode and MOSFET, the former as an essential element in NWFET and the latter as a general background of the FET. During this discussion, the photo-diode, solar cell, LED, LD, DRAM, flash EEPROM and sensors are highlighted to pave the way for similar applications of NWFET. Modeling is discussed in close analogy and comparison with MOSFETs. Contributors focus on processing, electrostatic discharge (ESD) and application of NWFET. This includes coverage of solar and memory cells, biological and chemical sensors, displays and atomic scale light emitting diodes. Appropriate for scientists and engineers interested in acquiring a working knowledge of NWFET as well as graduate students specializing in this subject.

**Modeling Materials** Ellad B. Tadmor, Ronald E. Miller. 2011-11-24 Material properties emerge from phenomena on scales ranging from Angstroms to millimeters, and only a multiscale treatment can provide a complete understanding. Materials researchers must therefore understand fundamental concepts and techniques from different fields, and these are presented in a comprehensive and integrated fashion for the first time in this book. Incorporating continuum mechanics, quantum mechanics, statistical mechanics, atomistic simulations and multiscale techniques, the book explains many of the key theoretical ideas behind multiscale modeling. Classical topics are blended with new techniques to demonstrate the connections between different fields and highlight current research trends. Example applications drawn from modern research on the thermo-mechanical properties of crystalline solids are used as a unifying focus throughout the text. Together with its companion book, *Continuum Mechanics and Thermodynamics* (Cambridge University Press, 2011), this work presents the complete fundamentals of materials modeling for graduate students and researchers in physics, materials science, chemistry and engineering.

Health and Environmental Safety of Nanomaterials James Njuguna, Krzysztof Pielichowski, Huijun Zhu. 2021-07-24 The first edition of *Health and Environmental Safety of Nanomaterials: Polymer Nanocomposites and Other Materials Containing Nanoparticles* was published in 2014, but since that time, new developments in the field of nanomaterials safety have emerged, both at release and exposure, along with the expanding applications of the nanomaterials side. Numerous studies have been dedicated to the issue of biophysical interactions of nanoparticles with the human body at the organ, cellular, and molecular levels. In this second edition, all the chapters have been brought fully up to date. There are also four brand new chapters on the biophysical interaction of nanoparticles with the human body; advanced modeling approaches to help elucidate the nanorisks; safety measures at work with nanoparticles; and the health and environmental risks of graphene. It provides key knowledge and information needs for all those who are working in the research and development sector and need to learn more about the safety of nanomaterials. • Focuses on the health and safety of polymer nanocomposites and other materials containing nanoparticles, as well as their medical and environmental implications • Discusses the fundamental nature of various biophysical interactions of nanoparticles with the human body • Looks at the physico-chemistry of nanoparticles and their uptake, translocation, transformation, transport, and biodistribution in mammalian and plant systems • Presents the structure-activity relationships and modeling of the interactions of nanoparticles with biological molecules, biochemical pathways, analysis of biomolecular signatures, and the development of biomarkers.

**Computational Materials System Design** Dongwon Shin, James Saal. 2017-11-10 This book provides state-of-the-art computational approaches for accelerating materials discovery, synthesis, and processing using thermodynamics and kinetics. The authors deliver an overview of current practical computational tools for materials design in the field. They describe ways to integrate thermodynamics and kinetics and how the two can supplement

each other.

**Fundamentals of Nanotransistors** Mark Lundstrom.2017-07-11 The transistor is the key enabler of modern electronics. Progress in transistor scaling has pushed channel lengths to the nanometer regime where traditional approaches to device physics are less and less suitable. These lectures describe a way of understanding MOSFETs and other transistors that is much more suitable than traditional approaches when the critical dimensions are measured in nanometers. It uses a novel, "bottom-up approach" that agrees with traditional methods when devices are large, but that also works for nano-devices. Surprisingly, the final result looks much like the traditional, textbook, transistor models, but the parameters in the equations have simple, clear interpretations at the nanoscale. The objective is to provide readers with an understanding of the essential physics of nanoscale transistors as well as some of the practical technological considerations and fundamental limits. This book is written in a way that is broadly accessible to students with only a very basic knowledge of semiconductor physics and electronic circuits. Complemented with online lecture by Prof Lundstrom: nanoHUB-U Nanoscale Transistor Contents:MOSFET Fundamentals:OverviewThe Transistor as a Black BoxThe MOSFET: A Barrier-Controlled DeviceMOSFET IV: Traditional ApproachMOSFET IV: The Virtual Source ModelMOS Electrostatics:Poisson Equation and the Depletion ApproximationGate Voltage and Surface PotentialMobile Charge: Bulk MOSMobile Charge: Extremely Thin SOI2D MOS ElectrostaticsThe VS Model RevisitedThe Ballistic MOSFET:The Landauer Approach to TransportThe Ballistic MOSFETThe Ballistic Injection VelocityConnecting the Ballistic and VS ModelsTransmission Theory of the MOSFET:Carrier Scattering and TransmissionTransmission Theory of the MOSFETConnecting the Transmission and VS ModelsVS Characterization of Transport in NanotransistorsLimits and Limitations Readership: Any student and professional with an undergraduate degree in the physical sciences or engineering.

*Electronic Density of States* Lawrence Herman Bennett.1971

*Quantum Wells, Wires and Dots* Paul Harrison.2005-10-31 Quantum Wells, Wires and Dots Second Edition: Theoretical andComputational Physics of Semiconductor Nanostructures providesall the essential information, both theoretical and computational,for complete beginners to develop an understanding of how theelectronic, optical and transport properties of quantum wells,wires and dots are calculated. Readers are lead through a series ofsimple theoretical and computational examples giving solidfoundations from which they will gain the confidence to initiate theoretical investigations or explanations of their own. Emphasis on combining the analysis and interpretation ofexperimental data with the development of theoretical ideas Complementary to the more standard texts Aimed at the physics community at large, rather than just the low-dimensional semiconductor expert The text present solutions for a large number of realsituations Presented in a lucid style with easy to follow steps related toaccompanying illustrative examples

Near-Equilibrium Transport Mark Lundstrom,Changwook Jeong.2012-11-29 These lectures are designed to introduce students to the fundamentals of carrier transport in nano-devices using a novel, "bottom up approach" that agrees with traditional methods when devices are large, but which also works for nano-devices. The goal is to help students learn how to think about carrier transport at the nanoscale and also how the bottom up approach provides a new perspective to traditional concepts like mobility and drift-diffusion equations. The lectures are designed for engineers and scientists and others who need a working knowledge of near-equilibrium ("low-field" or "linear") transport. Applications of the theory and measurement considerations are also addressed. The lectures serve as a starting point to an extensive set of instructional materials available online.

**Learning the Art of Electronics** Thomas C. Hayes,Paul Horowitz.2016-03-02 This introduction to circuit design is unusual in several respects. First, it offers not just explanations, but a full course. Each of the twenty-five sessions begins with a discussion of a particular sort of circuit followed by the chance to try it out and see how it actually behaves. Accordingly, students understand the circuit's operation in a way that is deeper and much

more satisfying than the manipulation of formulas. Second, it describes circuits that more traditional engineering introductions would postpone: on the third day, we build a radio receiver; on the fifth day, we build an operational amplifier from an array of transistors. The digital half of the course centers on applying microcontrollers, but gives exposure to Verilog, a powerful Hardware Description Language. Third, it proceeds at a rapid pace but requires no prior knowledge of electronics. Students gain intuitive understanding through immersion in good circuit design.

**Semiconductor Device Fundamentals** Robert F. Pierret.1996 Although roughly a half-century old, the field of study associated with semiconductor devices continues to be dynamic and exciting. New and improved devices are being developed at an almost frantic pace. While the number of devices in complex integrated circuits increases and the size of chips decreases, semiconductor properties are now being engineered to fit design specifications. Semiconductor Device Fundamentals serves as an excellent introduction to this fascinating field. Based in part on the Modular Series on Solid State Devices, this textbook explains the basic terminology, models, properties, and concepts associated with semiconductors and semiconductor devices. The book provides detailed insight into the internal workings of building block device structures and systematically develops the analytical tools needed to solve practical device problems.

**Green Technology for Smart City and Society** Renu Sharma,Manohar Mishra,Janmenjoy Nayak,Bighnaraj Naik,Danilo Pelusi.2020-11-30 This book includes selected papers from the International Conference on Green Technology for Smart City and Society (GTSCS 2020), organized by the Institute of Technical Education and Research, Siksha 'O' Anusandhan University, Bhubaneswar, India, during 13-14 August 2020. The book covers topics such as machine learning, artificial intelligence, deep learning, optimization algorithm, IoT, signal processing, etc. The book is helpful for researchers working in the discipline of Electrical, Electronics and Computer Science. The researchers working in the allied domain of communication and control will also find the book useful as it deals with the latest methodologies and applications.

Quantum Transport in Semiconductor Nanostructures Tillmann Christoph Kubis.2009

Compact Modeling Gennady Gildenblat.2010-06-22 Most of the recent texts on compact modeling are limited to a particular class of semiconductor devices and do not provide comprehensive coverage of the field. Having a single comprehensive reference for the compact models of most commonly used semiconductor devices (both active and passive) represents a significant advantage for the reader. Indeed, several kinds of semiconductor devices are routinely encountered in a single IC design or in a single modeling support group. Compact Modeling includes mostly the material that after several years of IC design applications has been found both theoretically sound and practically significant. Assigning the individual chapters to the groups responsible for the definitive work on the subject assures the highest possible degree of expertise on each of the covered models.

Junctionless Field-Effect Transistors Shubham Sahay,Mamidala Jagadesh Kumar.2019-01-28 A comprehensive one-volume reference on current JLFET methods, techniques, and research Advancements in transistor technology have driven the modern smart-device revolution—many cell phones, watches, home appliances, and numerous other devices of everyday usage now surpass the performance of the room-filling supercomputers of the past. Electronic devices are continuing to become more mobile, powerful, and versatile in this era of internet-of-things (IoT) due in large part to the scaling of metal-oxide semiconductor field-effect transistors (MOSFETs). Incessant scaling of the conventional MOSFETs to cater to consumer needs without incurring performance degradation requires costly and complex fabrication process owing to the presence of metallurgical junctions. Unlike conventional MOSFETs, junctionless field-effect transistors (JLFETs) contain no metallurgical junctions, so they are simpler to process and less costly to manufacture.JLFETs utilize a gated semiconductor film to control its resistance and the current flowing through it. Junctionless Field-Effect Transistors: Design, Modeling, and Simulation is an inclusive, one-stop reference on the study and research on JLFETs This timely book covers the fundamental physics underlying JLFET operation, emerging architectures, modeling and simulation methods, comparative analyses of JLFET

performance metrics, and several other interesting facts related to JLFETs. A calibrated simulation framework, including guidance on SentaurusTCAD software, enables researchers to investigate JLFETs, develop new architectures, and improve performance. This valuable resource: Addresses the design and architecture challenges faced by JLFET as a replacement for MOSFET Examines various approaches for analytical and compact modeling of JLFETs in circuit design and simulation Explains how to use Technology Computer-Aided Design software (TCAD) to produce numerical simulations of JLFETs Suggests research directions and potential applications of JLFETs Junctionless Field-Effect Transistors: Design, Modeling, and Simulation is an essential resource for CMOS device design researchers and advanced students in the field of physics and semiconductor devices.

**Nano-Electronic Devices** Dragica Vasileska, Stephen M. Goodnick. 2011-06-10 This book surveys the advanced simulation methods needed for proper modeling of state-of-the-art nanoscale devices. It systematically describes theoretical approaches and the numerical solutions that are used in explaining the operation of both power devices as well as nano-scale devices. It clearly explains for what types of devices a particular method is suitable, which is the most critical point that a researcher faces and has to decide upon when modeling semiconductor devices.

**Band Structure of Semiconductors** I. M. Tsidilkovski. 2016-10-19 Band Structure of Semiconductors provides a review of the theoretical and experimental methods of investigating band structure and an analysis of the results of the developments in this field. The book presents the problems, methods, and applications in the study of band structure. Topics on the computational methods of band structure; band structures of important semiconducting materials; behavior of an electron in a perturbed periodic field; effective masses and g-factors for the most commonly encountered band structures; and the treatment of cyclotron resonance, Shubnikov-de Haas oscillations, magnetophonon resonance, and magneto-optical phenomena are discussed. Experimental physicists, theoretical physicists, students and research workers, and engineers working in the field of semiconductor electronics will find this book a great source of vital information.

*12 Second Culture* Mike Metcalf, Shaun Peet. 2020-04-27

**2D Materials** Phaedon Avouris, Tony F. Heinz, Tony Low. 2017-06-29 Learn about the most recent advances in 2D materials with this comprehensive and accessible text. Providing all the necessary materials science and physics background, leading experts discuss the fundamental properties of a wide range of 2D materials, and their potential applications in electronic, optoelectronic and photonic devices. Several important classes of materials are covered, from more established ones such as graphene, hexagonal boron nitride, and transition metal dichalcogenides, to new and emerging materials such as black phosphorus, silicene, and germanene. Readers will gain an in-depth understanding of the electronic structure and optical, thermal, mechanical, vibrational, spin and plasmonic properties of each material, as well as the different techniques that can be used for their synthesis. Presenting a unified perspective on 2D materials, this is an excellent resource for graduate students, researchers and practitioners working in nanotechnology, nanoelectronics, nanophotonics, condensed matter physics, and chemistry.

**Ultrafast Optics** Andrew Weiner. 2011-09-20 A comprehensive treatment of ultrafast optics This book fills the need for a thorough and detailed account of ultrafast optics. Written by one of the most preeminent researchers in the field, it sheds new light on technology that has already had a revolutionary impact on precision frequency metrology, high-speed electrical testing, biomedical imaging, and in revealing the initial steps in chemical reactions. Ultrafast Optics begins with a summary of ultrashort laser pulses and their practical applications in a range of real-world settings. Next, it reviews important background material, including an introduction to Fourier series and Fourier transforms, and goes on to cover: Principles of mode-locking Ultrafast pulse measurement methods Dispersion and dispersion compensation Ultrafast nonlinear optics: second order Ultrafast nonlinear optics: third order Mode-locking: selected advanced topics Manipulation of ultrashort pulses Ultrafast time-resolved spectroscopy

Terahertz time-domain electromagnetics Professor Weiner's expertise and cutting-edge research result in a book that is destined to become a seminal text for engineers, researchers, and graduate students alike.

**Nanoelectronic Device Applications Handbook** James E. Morris, Krzysztof Iniewski. 2017-11-22 Nanoelectronic Device Applications Handbook gives a comprehensive snapshot of the state of the art in nanodevices for nanoelectronics applications. Combining breadth and depth, the book includes 68 chapters on topics that range from nano-scaled complementary metal-oxide-semiconductor (CMOS) devices through recent developments in nano capacitors and AlGaAs/GaAs devices. The contributors are world-renowned experts from academia and industry from around the globe. The handbook explores current research into potentially disruptive technologies for a post-CMOS world. These include: Nanoscale advances in current MOSFET/CMOS technology Nano capacitors for applications such as electronics packaging and humidity sensors Single electron transistors and other electron tunneling devices Quantum cellular automata and nanomagnetic logic Memristors as switching devices and for memory Graphene preparation, properties, and devices Carbon nanotubes (CNTs), both single CNT and random network Other CNT applications such as terahertz, sensors, interconnects, and capacitors Nano system architectures for reliability Nanowire device fabrication and applications Nanowire transistors Nanodevices for spintronics The book closes with a call for a new generation of simulation tools to handle nanoscale mechanisms in realistic nanodevice geometries. This timely handbook offers a wealth of insights into the application of nanoelectronics. It is an invaluable reference and source of ideas for anyone working in the rapidly expanding field of nanoelectronics.

Thermoelectric Energy Conversion Devices And Systems Kazuaki Yazawa, Je-hyeong Bahk, Ali Shakouri. 2021-02-23 This unique compendium emphasizes key factors driving the performance of thermoelectric energy conversion systems. Important design parameters such as heat transfer at the boundaries of the system, material properties, and form factors are carefully analyzed and optimized for performance including the cost-performance trade-off. Numbers of examples are provided on the applications of thermoelectric technologies, e.g., power generation, cooling of electronic components, and waste heat recovery in wearable devices. This must-have volume also includes an interactive modeling software package developed on the nanoHUB (<https://nanohub.org/>) platform. Professionals, researchers, academics, undergraduate and graduate students will be able to study the impact of material properties and key design parameters on the overall thermoelectric system performance as well as the large scale implementation in the society.

**Multiscale Modeling of Complex Molecular Structure and Dynamics with MBN Explorer** Ilia A. Solov'yov, Andrey V. Korol, Andrey V. Solov'yov. 2017-05-16 This book introduces readers to MesoBioNano (MBN) Explorer - a multi-purpose software package designed to model molecular systems at various levels of size and complexity. In addition, it presents a specially designed multi-task toolkit and interface - the MBN Studio - which enables the set-up of input files, controls the simulations, and supports the subsequent visualization and analysis of the results obtained. The book subsequently provides a systematic description of the capabilities of this universal and powerful software package within the framework of computational molecular science, and guides readers through its applications in numerous areas of research in bio- and chemical physics and material science - ranging from the nano- to the mesoscale. MBN Explorer is particularly suited to computing the system's energy, to optimizing molecular structure, and to exploring the various facets of molecular and random walk dynamics. The package allows the use of a broad variety of interatomic potentials and can, e.g., be configured to select any subset of a molecular system as rigid fragments, whenever a significant reduction in the number of dynamical degrees of freedom is required for computational practicalities. MBN Studio enables users to easily construct initial geometries for the molecular, liquid, crystalline, gaseous and hybrid systems that serve as input for the subsequent simulations of their physical and chemical properties using MBN Explorer. Despite its universality, the computational efficiency of MBN Explorer is comparable to that of

other, more specialized software packages, making it a viable multi-purpose alternative for the computational modeling of complex molecular systems. A number of detailed case studies presented in the second part of this book demonstrate MBN Explorer's usefulness and efficiency in the fields of atomic clusters and nanoparticles, biomolecular systems, nanostructured materials, composite materials and hybrid systems, crystals, liquids and gases, as well as in providing modeling support for novel and emerging technologies. Last but not least, with the release of the 3rd edition of MBN Explorer in spring 2017, a free trial version will be available from the MBN Research Center website ([mbnresearch.com](http://mbnresearch.com)).

*Electronic Structure* Richard M. Martin.2004-04-08 The study of the electronic structure of materials is at a momentous stage, with the emergence of computational methods and theoretical approaches. Many properties of materials can now be determined directly from the fundamental equations for the electrons, providing insights into critical problems in physics, chemistry, and materials science. This book provides a unified exposition of the basic theory and methods of electronic structure, together with instructive examples of practical computational methods and real-world applications. Appropriate for both graduate students and practising scientists, this book describes the approach most widely used today, density functional theory, with emphasis upon understanding the ideas, practical methods and limitations. Many references are provided to original papers, pertinent reviews, and widely available books. Included in each chapter is a short list of the most relevant references and a set of exercises that reveal salient points and challenge the reader.

**Electronic Transport in Mesoscopic Systems** Supriyo Datta.1997-05-15 Advances in semiconductor technology have made possible the fabrication of structures whose dimensions are much smaller than the mean free path of an electron. This book gives a thorough account of the theory of electronic transport in such mesoscopic systems. After an initial chapter covering fundamental concepts, the transmission function formalism is presented, and used to describe three key topics in mesoscopic physics: the quantum Hall effect; localisation; and double-barrier tunnelling. Other sections include a discussion of optical analogies to mesoscopic phenomena, and the book concludes with a description of the non-equilibrium Green's function formalism and its relation to the transmission formalism. Complete with problems and solutions, the book will be of great interest to graduate students of mesoscopic physics and nanoelectronic device engineering, as well as to established researchers in these fields.

Nano/Microscale Heat Transfer Zhuomin M. Zhang.2020-06-23 This substantially updated and augmented second edition adds over 200 pages of text covering and an array of newer developments in nanoscale thermal transport. In *Nano/Microscale Heat Transfer*, 2nd edition, Dr. Zhang expands his classroom-proven text to incorporate thermal conductivity spectroscopy, time-domain and frequency-domain thermoreflectance techniques, quantum size effect on specific heat, coherent phonon, minimum thermal conductivity, interface thermal conductance, thermal interface materials, 2D sheet materials and their unique thermal properties, soft materials, first-principles simulation, hyperbolic metamaterials, magnetic polaritons, and new near-field radiation experiments and numerical simulations. Informed by over 12 years use, the author's research experience, and feedback from teaching faculty, the book has been reorganized in many sections and enriched with more examples and homework problems. Solutions for selected problems are also available to qualified faculty via a password-protected website. • Substantially updates and augments the widely adopted original edition, adding over 200 pages and many new illustrations; • Incorporates student and faculty feedback from a decade of classroom use; • Elucidates concepts explained with many examples and illustrations; • Supports student application of theory with 300 homework problems; • Maximizes reader understanding of micro/nanoscale thermophysical properties and processes and how to apply them to thermal science and engineering; • Features MATLAB codes for working with size and temperature effects on thermal conductivity, specific heat of nanostructures, thin-film optics, RCWA, and near-field radiation.



*The Physics of Graphene* Mikhail I. Katsnelson.2020-03-19 Leading graphene research theorist Mikhail I. Katsnelson systematically presents the basic concepts of graphene physics in this fully revised second edition. The author illustrates and explains basic concepts such as Berry phase, scaling, Zitterbewegung, Kubo, Landauer and Mori formalisms in quantum kinetics, chirality, plasmons, commensurate-incommensurate transitions and many others. Open issues and unsolved problems introduce the reader to the latest developments in the field. New achievements and topics presented include the basic concepts of Van der Waals heterostructures, many-body physics of graphene, electronic optics of Dirac electrons, hydrodynamics of electron liquid and the mechanical properties of one atom-thick membranes. Building on an undergraduate-level knowledge of quantum and statistical physics and solid-state theory, this is an important graduate textbook for students in nanoscience, nanotechnology and condensed matter. For physicists and material scientists working in related areas, this is an excellent introduction to the fast-growing field of graphene science.

*Electronic Structure and the Properties of Solids* Walter A. Harrison.2012-03-08 This text offers basic understanding of the electronic structure of covalent and ionic solids, simple metals, transition metals and their compounds; also explains how to calculate dielectric, conducting, bonding properties.

*International Assessment of Research and Development in Simulation-based Engineering and Science* Sharon C. Glotzer,National Science Foundation (U.S.).2011 Simulation-Based Engineering and Science (SBE&S) cuts across disciplines, showing tremendous promise in areas from storm prediction and climate modeling to understanding the brain and the behavior of numerous other complex systems. In this groundbreaking volume, nine distinguished leaders assess the latest research trends, as a result of 52 site visits in Europe and Asia and hundreds of hours of expert interviews, and discuss the implications of their findings for the US government. The authors conclude that while the US remains the quantitative leader in SBE&S research and development, it is very much in danger of losing that edge to Europe and Asia. Commissioned by the National Science Foundation, this multifaceted study will capture the attention of Fortune 500 companies and policymakers.

**Thermally-Aware Design** Yong Zhan,Sanjay V. Kumar,Sachin S. Sapatnekar.2008 Provides an overview of analysis and optimization techniques for thermally-aware chip design.

*Coherent Nonlinear Optics* M.S. Feld,V.S. Letokhov.2012-12-06

Whispering the Strategies of Language: An Emotional Quest through **Electronic Band Structure Calculation Nanohub Org Home**

In a digitally-driven world wherever screens reign supreme and instant interaction drowns out the subtleties of language, the profound techniques and psychological subtleties hidden within phrases frequently move unheard. However, set within the pages of **Electronic Band Structure Calculation Nanohub Org Home** a captivating fictional prize blinking with organic thoughts, lies an extraordinary journey waiting to be undertaken. Penned by an experienced wordsmith, that wonderful opus encourages visitors on an introspective trip, lightly unraveling the veiled truths and profound affect resonating within the very material of each word. Within the mental depths of the poignant evaluation, we shall embark upon a sincere exploration of the book's key subjects, dissect its fascinating writing model, and yield to the effective resonance it evokes deep within the recesses of readers hearts.

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