Computational Electronics Semiclassical And Quantum Device Modeling And Simulation | 90dbcee7832c3350b7f7e9db57ac17b3

Computational ElectronicsComputational ElectronicsExploring the QuantumPrinciples and Applications of Quantum ChemistryNano-Electronic DevicesClassical and Quantum Dynamics in Condensed Phase SimulationsICT Innovations 2009The Semiclassical Way to Dynamics and SpectroscopyComputational PhotochemistryIntroduction to Quantum Electronics and Nonlinear OpticsIntroduction to Quantum OpticsNano-Electronic DevicesModeling Self-Heating Effects in Nanoscale DevicesQuantum ChaosAn Introduction to Quantum ComputingPrinciples of Data ScienceTunnelling in MoleculesNanoscale MOS TransistorsSolid State TheoryComputational ElectronicsSemiclassical and Stochastic GravityQuantum TransportQuantum OpticsNanoelectronic Device Applications HandbookElectron Phonon InteractionsPhoton-Atom InteractionsMathematical Challenges from Theoretical/Computational ChemistryThe Non-Equilibrium Green's Function Method for Nanoscale Device SimulationElectronic Quantum Transport in Mesoscopic Semiconductor StructuresQuantum Computing and Quantum CommunicationsNanophononicsThe Physics of Solar CellsQuantum-Based Electronic Devices and SystemsHandbook of Optoelectronic Device Modeling and SimulationQuantum ComputingLarge-scale Simulations of Error Prone Quantum Computation DevicesQuantum Chemistry and Dynamics of Excited StatesCoherent Raman Scattering MicroscopyQuantum Algorithms Via Linear AlgebraElectrically Driven Quantum Dot Based Single-Photon Sources

Computational Electronics

An introduction to the rapidly evolving methodology of electronic excited states For academic researchers, postdocs, graduate and undergraduate students, Quantum Chemistry and Dynamics of Excited States: Methods and Applications reports the most updated and accurate theoretical techniques to treat electronic excited states.

From methods to deal with stationary calculations through time-dependent simulations of molecular systems, this book serves as a guide for beginners in the field and knowledge seekers alike. Taking into account the most recent theory developments and representative applications, it also covers the often-overlooked gap between theoretical and computational chemistry. An excellent reference for both researchers and students, Excited States provides essential knowledge on quantum chemistry, an in-depth overview of the latest developments, and theoretical techniques around the properties and nonadiabatic dynamics of chemical systems. Readers will learn: ⬮ Essential theoretical techniques to describe the properties and dynamics of chemical systems ⬮ Electronic Structure methods for stationary calculations ⬮ Methods for electronic excited states from both a quantum chemical and time-dependent point of view ⬮ A breakdown of the most recent developments in the past 30 years For those searching for a better understanding of excited states as they relate to chemistry, biochemistry, industrial chemistry, and beyond, Quantum Chemistry and Dynamics of Excited States provides a solid education in the necessary foundations and important theories of excited states in photochemistry and ultrafast phenomena.

Computational Electronics

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.

Exploring the Quantum

Principles and Applications of Quantum Chemistry

A graduate-level text that examines the semiclassical approach to quantum mechanics Physical systems have been traditionally described in terms of either classical or quantum mechanics. But in recent years, semiclassical methods have developed rapidly, providing deep physical insight and computational tools for quantum dynamics and spectroscopy. In this book, Eric Heller introduces and develops this subject, demonstrating its power with many examples. In the first half of the book, Heller covers relevant aspects of classical mechanics, building from them the semiclassical way through the semiclassical limit of the Feynman path integral. The second half of the book applies this approach to various kinds of spectroscopy, such as molecular spectroscopy and electron imaging and quantum dynamical systems with an emphasis on tunneling. Adopting a distinctly time-dependent viewpoint, Heller argues for semiclassical theories from experimental and theoretical vantage points valuable to research in physics and chemistry. Featuring more than two hundred figures, the book provides a geometric, phase-space, and coordinate-space pathway to greater understanding. Filled with practical examples and applications, The Semiclassical Way to Dynamics and Spectroscopy is a comprehensive presentation of the tools necessary to successfully delve into this unique area of quantum mechanics. A comprehensive approach for using classical mechanics to do quantum mechanics More than two hundred figures to assist intuition Emphasis on semiclassical Green function and wave packet perspective, as well as tunneling and spectroscopy Chapters include quantum mechanics of classically chaotic systems, quantum scarring, and other modern dynamical topics

Nano-Electronic Devices

Quantum transport is a diverse field, sometimes combining seemingly contradicting concepts - quantum and classical, conduction and insulating - within a single nanodevice. Quantum transport is an essential and challenging part of nanoscience, and understanding its concepts and methods is vital to the successful fabrication of devices at the nanoscale. This textbook is a comprehensive introduction to the rapidly developing field of quantum transport. The authors present the comprehensive theoretical background, and explore the groundbreaking experiments that laid the foundations of the field. Ideal for graduate students, each section contains control questions and exercises to check readers' understanding of the topics covered. Its broad scope

and in-depth analysis of selected topics will appeal to researchers and professionals working in nanoscience.

Classical and Quantum Dynamics in Condensed Phase Simulations

Written from an engineering standpoint, this book provides the theoretical background and physical insight needed to understand new and future developments in the modeling and design of n- and p-MOS nanoscale transistors. A wealth of applications, illustrations and examples connect the methods described to all the latest issues in nanoscale MOSFET design. Key areas covered include: • Transport in arbitrary crystal orientations and strain conditions, and new channel and gate stack materials • All the relevant transport regimes, ranging from low field mobility to quasi-ballistic transport, described using a single modeling framework • Predictive capabilities of device models, discussed with systematic comparisons to experimental results

ICT Innovations 2009

The First Book on CRS Microscopy Compared to conventional Raman microscopy, coherent Raman scattering (CRS) allows label-free imaging of living cells and tissues at video rate by enhancing the weak Raman signal through nonlinear excitation. Edited by pioneers in the field and with contributions from a distinguished team of experts, Coherent Raman Scattering Microscopy explains how CRS can be used to obtain a point-by-point chemical map of live cells and tissues. In color throughout, the book starts by establishing the foundation of CRS microscopy. It discusses the principles of nonlinear optical spectroscopy, particularly coherent Raman spectroscopy, and presents the theories of contrast mechanisms pertinent to CRS microscopy. The text then provides important technical aspects of CRS microscopy, including microscope construction, detection schemes, and data analyses. It concludes with a survey of applications that demonstrate how CRS microscopy has become a valuable tool in biomedicine. Due to its label-free, noninvasive examinations of living cells and organisms, CRS microscopy has opened up exciting prospects in biology and medicine—from the mapping of 3D distributions of small drug molecules to identifying tumors in tissues. An in-depth exploration of the theories, technology, and

applications, this book shows how CRS microscopy has impacted human health and will deepen our understanding of life processes in the future.

The Semiclassical Way to Dynamics and Spectroscopy

Quantum computing explained in terms of elementary linear algebra, emphasizing computation and algorithms and requiring no background in physics.

Computational Photochemistry

This textbook, based on the authors' class-tested material, is accessible to students at the advanced undergraduate and graduate level in physics and engineering. While its primary function is didactic, this book's comprehensive choice of topics and its clear and authoritative synthesis of ideas make it a useful reference for researchers, device engineers, and course instructors who wish to consolidate their knowledge of this field. The book takes the semi-classical approach where light is treated as a wave in accordance with the classical Maxwell equations, while matter is governed by quantum theory. It begins by introducing the postulates and mathematical framework of quantum theory, followed by the formalism of the density matrix which allows the transition from microscopic (quantum) quantities to macroscopic (classical) ones. Consequently, the equations describing the reaction of matter to the electromagnetic field in the form of polarization, magnetization, and current are derived. These equations (together with the Maxwell equations) form the complete system of equations sufficient to model a wide class of problems surrounding linear and nonlinear interactions of electromagnetic fields with matter. The nonlinear character of the governing equations determines parameters of the steady-state mode of the quantum generator and is also demonstrated in harmonic generation via propagation of laser radiation in various media. The touchstone description of magnetic phenomena will be of interest to scientists who deal with applications of magneto-resonance phenomena in biology and medicine. Other advanced topics covered include electric dipole transitions, magnetic dipole transitions, plasma transitions, and the devices that can be based on these and other

electro-optical and nonlinear-optical systems. This textbook features numerous exercises, some of which are investigatory and some of which require computational solutions.

Introduction to Quantum Electronics and Nonlinear Optics

Starting with the simplest semiclassical approaches and ending with the description of complex fully quantum-mechanical methods for quantum transport analysis of state-of-the-art devices, Computational Electronics: Semiclassical and Quantum Device Modeling and Simulation provides a comprehensive overview of the essential techniques and methods for effectively analyzing transport in semiconductor devices. With the transistor reaching its limits and new device designs and paradigms of operation being explored, this timely resource delivers the simulation methods needed to properly model state-of.

Introduction to Quantum Optics

Heat in most semiconductor materials, including the traditional group IV elements (Si, Ge, diamond), III – V compounds (GaAs, wide-bandgap GaN), and carbon allotropes (graphene, CNTs), as well as emerging new materials like transition metal dichalcogenides (TMDCs), is stored and transported by lattice vibrations (phonons). Phonon generation through interactions with electrons (in nanoelectronics, power, and nonequilibrium devices) and light (optoelectronics) is the central mechanism of heat dissipation in nanoelectronics. This book focuses on the area of thermal effects in nanostructures, including the generation, transport, and conversion of heat at the nanoscale level. Phonon transport, including thermal conductivity in nanostructured materials, as well as numerical simulation methods, such as phonon Monte Carlo, Green's functions, and first principles methods, feature prominently in the book, which comprises four main themes: (i) phonon generation/heat dissipation, (i) nanoscale phonon transport, (iii) applications/devices (including thermoelectrics), and (iv) emerging materials (graphene/2D). The book also covers recent advances in nanophononics—the study of phonons at the nanoscale. Applications of nanophononics focus on thermoelectric (TE) and tandem TE/photovoltaic energy conversion. The

applications are augmented by a chapter on heat dissipation and self-heating in nanoelectronic devices. The book concludes with a chapter on thermal transport in nanoscale graphene ribbons, covering recent advances in phonon transport in 2D materials. The book will be an excellent reference for researchers and graduate students of nanoelectronics, device engineering, nanoscale heat transfer, and thermoelectric energy conversion. The book could also be a basis for a graduate special topics course in the field of nanoscale heat and energy.

Nano-Electronic Devices

Starting with the simplest semiclassical approaches and ending with the description of complex fully quantum-mechanical methods for quantum transport analysis of state-of-the-art devices, Computational Electronics: Semiclassical and Quantum Device Modeling and Simulation provides a comprehensive overview of the essential techniques and methods for effectively analyzing transport in semiconductor devices. With the transistor reaching its limits and new device designs and paradigms of operation being explored, this timely resource delivers the simulation methods needed to properly model state-of-the-art nanoscale devices. The first part examines semiclassical transport methods, including drift-diffusion, hydrodynamic, and Monte Carlo methods for solving the Boltzmann transport equation. Details regarding numerical implementation and sample codes are provided as templates for sophisticated simulation software. The second part introduces the density gradient method, quantum hydrodynamics, and the concept of effective potentials used to account for quantum-mechanical space quantization effects in particle-based simulators. Highlighting the need for quantum transport approaches, it describes various quantum effects that appear in current and future devices being mass-produced or fabricated as a proof of concept. In this context, it introduces the concept of effective potential used to approximately include quantum-mechanical space-quantization effects within the semiclassical particle-based device simulation scheme. Addressing the practical aspects of computational electronics, this authoritative resource concludes by addressing some of the open questions related to quantum transport not covered in most books. Complete with self-study problems and numerous examples throughout, this book supplies readers with the practical understanding required to create their own simulators.

Modeling Self-Heating Effects in Nanoscale Devices

This monograph is a radical departure from the conventional quantum mechanical approach to electron-phonon interactions. It translates the customary quantum mechanical analysis of the electron-phonon interactions carried out in Fourier space into a predominantly classical analysis carried out in real space. Various electron-phonon interactions such as the polar and nonpolar optical phonons, acoustic phonons that interact via deformation potential and via the piezoelectric effect and phonons in metals, are treated in this monograph by a single, relatively simple ?classical? model. This model is shown to apply to electron interactions with the deep lying X-ray levels of atoms, with plasmons and with Cerenkov radiation. The unifying concept that applies to all of these phenomena is a new definition of a coupling constant. The essentially classical interaction of an electron with its surrounding is clearly brought out to be the cause of spontaneous emission of phonons. The same concept also applies to the case of spontaneous emission of photons. While the bulk of this monograph deals with quanta of phonons and quanta of photons, a discussion of the acousto electric effect which is a purely classical phenomenon is presented. The newly defined coupling constant turns out to be valid too for this discussion. This universality of the coupling constant goes far beyond. It is equally applicable to amorphous materials. This significant application gives an analytic formulation of mobility in amorphous materials.

Quantum Chaos

An introduction to the physics of the photovoltaic cell. It covers the fundamental principles of semiconductor physics and simple models used to describe solar cell operation. It presents theoretical approaches to efficient solar cell design and examines the main practical types of solar cell

An Introduction to Quantum Computing

This book provides readers with a thorough understanding of various research areas within the field of data

science. The book introduces readers to various techniques for data acquisition, extraction, and cleaning, data summarizing and modeling, data analysis and communication techniques, data science tools, deep learning, and various data science applications. Researchers can extract and conclude various future ideas and topics that could result in potential publications or thesis. Furthermore, this book contributes to Data Scientists' preparation and to enhancing their knowledge of the field. The book provides a rich collection of manuscripts in highly regarded data science topics, edited by professors with long experience in the field of data science. Introduces various techniques, methods, and algorithms adopted by Data Science experts Provides a detailed explanation of data science perceptions, reinforced by practical examples Presents a road map of future trends suitable for innovative data science research and practice

Principles of Data Science

Computational Photochemistry, Volume 16 provides an overview of general strategies currently used to investigate photochemical processes. Whilst contributing to establishing a branch of computational chemistry that deals with the properties and reactivity of photoexcited molecules, the book also provides insight into the conceptual and methodological research lines in computational photochemistry. Packed with examples of applications of modelling of basic photochemical reactions and the computer-aided development of novel materials in the field of photodegradation (paints), photoprotection (sunscreens), color regulation (photochromic devices) and fluorescent probes, this book is particularly useful to anyone interested in the effect of light on molecules and materials. * Provides an overview of computational photochemistry, dealing with principles and applications * Demonstrates techniques that can be used in the computer-aided design of novel photo responsive materials * Written by experts in computational photochemistry

Tunnelling in Molecules

This book is the result of the first International Conference ICT Innovations 2009. The ICT Innovations conference

is the primary scientific action of the Macedonian Society on Information and Communication Technologies (ICT-ACT). It promotes the publication of scientific results of the international community related to innovative fundamental and applied research in ICT. Today, ICT has enlarged its horizons and it is practiced under multidisciplinary contexts that introduce new challenges to theore- cal and technical approaches. The ICT Innovations 2009 conference gathered academics, professionals and pr- titioners reporting their valuable experiences in developing solutions and systems in the industrial and business arena especially innovative commercial implementations, novel applications of technology, and experience in applying recent research advances to practical situations, in any ICT areas. The conference focuses on issues concerning a variety of ICT fields like: • Multimedia Information Systems • Artificial Intelligence • Pervasive and Ubiquitous Computing • Eco and Bio Informatics • Internet and Web Applications and Services • Wireless and Mobile Communications and Services • Computer Networks, Security and Cryptography • Distributed Systems, GRID and Cloud Computing ICT Innovations 2009 Conference was held in Ohrid, Macedonia, in September 28-30, 2009. Local arrangements provided by the members of the Macedonian Society on Information and Communication Technologies – ICT-ACT, mainly consisting of teaching and research staff of Computer Science Department at Faculty of Electrical Engineering and Information Technologies and Institute of Informatics at Faculty of Natural Sciences, both at Ss. Cyril and Methodius University in Skopje, Macedonia.

Nanoscale MOS Transistors

Quantum tunnelling is one of the strangest phenomena in chemistry, where we see the wave nature of atoms acting in “impossible” ways. By letting molecules pass through the kinetic barrier instead of over it, this effect can lead to chemical reactions even close to the absolute zero, to atypical spectroscopic observations, to bizarre selectivity, or to colossal isotopic effects. Quantum mechanical tunnelling observations might be infrequent in chemistry, but it permeates through all its disciplines producing remarkable chemical outcomes. For that reason, the 21st century has seen a great increase in theoretical and experimental findings involving molecular tunnelling effects, as well as in novel techniques that permit their accurate predictions and analysis. Including experimental,

computational and theoretical chapters, from the physical and organic to the biochemistry fields, from the applied to the academic arenas, this new book provides a broad and conceptual perspective on tunnelling reactions and how to study them. Quantum Tunnelling in Molecules is the obligatory stop for both the specialist and those new to this world.

Solid State Theory

Optoelectronic devices are now ubiquitous in our daily lives, from light emitting diodes (LEDs) in many household appliances to solar cells for energy. This handbook shows how we can probe the underlying and highly complex physical processes using modern mathematical models and numerical simulation for optoelectronic device design, analysis, and performance optimization. It reflects the wide availability of powerful computers and advanced commercial software, which have opened the door for non-specialists to perform sophisticated modeling and simulation tasks. The chapters comprise the know-how of more than a hundred experts from all over the world. The handbook is an ideal starting point for beginners but also gives experienced researchers the opportunity to renew and broaden their knowledge in this expanding field.

Computational Electronics

Starting with the simplest semiclassical approaches and ending with the description of complex fully quantum-mechanical methods for quantum transport analysis of state-of-the-art devices, Computational Electronics: Semiclassical and Quantum Device Modeling and Simulation provides a comprehensive overview of the essential techniques and methods for effectively analyzing transport in semiconductor devices. With the transistor reaching its limits and new device designs and paradigms of operation being explored, this timely resource delivers the simulation methods needed to properly model state-of-the-art nanoscale devices. The first part examines semiclassical transport methods, including drift-diffusion, hydrodynamic, and Monte Carlo methods for solving the Boltzmann transport equation. Details regarding numerical implementation and sample codes are provided as

templates for sophisticated simulation software. The second part introduces the density gradient method, quantum hydrodynamics, and the concept of effective potentials used to account for quantum-mechanical space quantization effects in particle-based simulators. Highlighting the need for quantum transport approaches, it describes various quantum effects that appear in current and future devices being mass-produced or fabricated as a proof of concept. In this context, it introduces the concept of effective potential used to approximately include quantum-mechanical space-quantization effects within the semiclassical particle-based device simulation scheme. Addressing the practical aspects of computational electronics, this authoritative resource concludes by addressing some of the open questions related to quantum transport not covered in most books. Complete with self-study problems and numerous examples throughout, this book supplies readers with the practical understanding required to create their own simulators.

Semiclassical and Stochastic Gravity

The authors provide an introduction to quantum computing. Aimed at advanced undergraduate and beginning graduate students in these disciplines, this text is illustrated with diagrams and exercises.

Quantum Transport

The school held at Villa Marigola, Lerici, Italy, in July 1997 was very much an educational experiment aimed not just at teaching a new generation of students the latest developments in computer simulation methods and theory, but also at bringing together researchers from the condensed matter computer simulation community, the biophysical chemistry community and the quantum dynamics community to confront the shared problem: the development of methods to treat the dynamics of quantum condensed phase systems. This volume collects the lectures delivered there. Due to the focus of the school, the contributions divide along natural lines into two broad groups: (1) the most sophisticated forms of the art of computer simulation, including biased phase space sampling schemes, methods which address the multiplicity of time scales in condensed phase problems, and static

equilibrium methods for treating quantum systems; (2) the contributions on quantum dynamics, including methods for mixing quantum and classical dynamics in condensed phase simulations and methods capable of treating all degrees of freedom quantum-mechanically. Contents:Barrier Crossing: Classical Theory of Rare but Important Events (D Chandler)Monte Carlo Simulations (D Frenkel)Molecular Dynamics Methods for the Enhanced Sampling of Phase Space (B J Berne)Constrained and Nonequilibrium Molecular Dynamics (G Ciccotti & M Ferrario)From Erying to Kramers: Computation of Diffusive Barrier Crossing Rates (M J Ruiz-Montero)Monte Carlo Methods for Sampling of Rare Event States (W Janke)Proton Transfer in Ice (D Marx)Nudged Elastic Band Method for Finding Minimum Energy Paths of Transitions (H J ó nsson et al.)RAW Quantum Transition State Theory (G Mills et al.)Dynamics of Peptide Folding (R Elber et al.)Theoretical Studies of Activated Processes in Biological Ion Channels (B Roux & S Crouzy)The Semiclassical Initial Value Representation for Including Quantum Effects in Molecular Dynamics Simulations (W H Miller)Tunneling in the Condensed Phase: Barrier Crossing and Dynamical Control (N Makri)Feynman Path Centroid Methods for Condensed Phase Quantum Dynamics (G A Voth)Quantum Molecular Dynamics Using Wigner Representation (V S Filinov et al.)Nonadiabatic Molecular Dynamics Methods for Diffusion (D Laria et al.)and other papers Readership: Computational and statistical physicists. Keywords:Quantum;Molecular Dynamics;DynamicsReviews: “… this volume is a useful introduction to currently popular, and widely-used techniques in chemical and statistical physics. The authors are well-respected researchers in the field and the level is appropriate to graduate students and researchers.” Journal of Statistical Physics

Quantum Optics

This book provides an introduction to the body of theory shared by several branches of modern optics--nonlinear optics, quantum electronics, laser physics, and quantum optics--with an emphasis on quantum and statistical aspects. It is intended for well prepared undergraduate and graduate students in physics, applied physics, electrical engineering, and chemistry who seek a level of preparation of sufficient maturity to enable them to follow the specialized literature.

Nanoelectronic Device Applications Handbook

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.

Electron Phonon Interactions

For modeling the transport of carriers in nanoscale devices, a Green-function formalism is the most accurate approach. Due to the complexity of the formalism, one should have a deep understanding of the underlying principles and use smart approximations and numerical methods for solving the kinetic equations at a reasonable computational time. In this book the required concepts from quantum and statistical mechanics and numerical methods for calculating Green functions are presented. The Green function is studied in detail for systems both under equilibrium and under nonequilibrium conditions. Because the formalism enables rigorous modeling of

different scattering mechanisms in terms of self-energies, but an exact evaluation of self-energies for realistic systems is not possible, their approximation and inclusion in the quantum kinetic equations of the Green functions are elaborated. All the elements of the kinetic equations, which are the device Hamiltonian, contact self-energies and scattering self-energies, are examined and efficient methods for their evaluation are explained. Finally, the application of these methods to study novel electronic devices such as nanotubes, graphene, Si-nanowires and low-dimensional thermoelectric devices and photodetectors are discussed.

Photon-Atom Interactions

It is generally acknowledged that modeling and simulation are preferred alternatives to trial and error approaches to semiconductor fabrication in the present environment, where the cost of process runs and associated mask sets is increasing exponentially with successive technology nodes. Hence, accurate physical device simulation tools are essential to accurately predict device and circuit performance. Accurate thermal modelling and the design of microelectronic devices and thin film structures at the micro- and nanoscales poses a challenge to electrical engineers who are less familiar with the basic concepts and ideas in sub-continuum heat transport. This book aims to bridge that gap. Efficient heat removal methods are necessary to increase device performance and device reliability. The authors provide readers with a combination of nanoscale experimental techniques and accurate modelling methods that must be employed in order to determine a device's temperature profile.

Mathematical Challenges from Theoretical/Computational Chemistry

Discusses quantum chaos, an important area of nonlinear science.

The Non-Equilibrium Green's Function Method for Nanoscale Device Simulation

DIVThorough, modern study of solid state physics; solid types and symmetry, electron states, electronic

properties and cooperative phenomena. /div

Electronic Quantum Transport in Mesoscopic Semiconductor Structures

The quantum world obeys logic at odds with our common sense intuition. This weirdness is directly displayed in recent experiments juggling with isolated atoms and photons. They are reviewed in this book, combining theoretical insight and experimental description, and providing useful illustrations for learning and teaching of quantum mechanics.

Quantum Computing and Quantum Communications

Covering a number of important subjects in quantum optics, this textbook is an excellent introduction for advanced undergraduate and beginning graduate students, familiarizing readers with the basic concepts and formalism as well as the most recent advances. The first part of the textbook covers the semi-classical approach where matter is quantized, but light is not. It describes significant phenomena in quantum optics, including the principles of lasers. The second part is devoted to the full quantum description of light and its interaction with matter, covering topics such as spontaneous emission, and classical and non-classical states of light. An overview of photon entanglement and applications to quantum information is also given. In the third part, non-linear optics and laser cooling of atoms are presented, where using both approaches allows for a comprehensive description. Each chapter describes basic concepts in detail, and more specific concepts and phenomena are presented in 'complements'.

Nanophononics

Principles and Applications of Quantum Chemistry offers clear and simple coverage based on the author’s extensive teaching at advanced universities around the globe. Where needed, derivations are detailed in an easy-

to-follow manner so that you will understand the physical and mathematical aspects of quantum chemistry and molecular electronic structure. Building on this foundation, this book then explores applications, using illustrative examples to demonstrate the use of quantum chemical tools in research problems. Each chapter also uses innovative problems and bibliographic references to guide you, and throughout the book chapters cover important advances in the field including: Density functional theory (DFT) and time-dependent DFT (TD-DFT), characterization of chemical reactions, prediction of molecular geometry, molecular electrostatic potential, and quantum theory of atoms in molecules. Simplified mathematical content and derivations for reader understanding Useful overview of advances in the field such as Density Functional Theory (DFT) and Time-Dependent DFT (TD-DFT) Accessible level for students and researchers interested in the use of quantum chemistry tools

The Physics of Solar Cells

This exhaustive survey of advanced simulation methods for modeling nanoscale devices systematically covers both theoretical approaches and numerical solutions, links methodology with the type of device, and includes advice on state-of-the-art semiconductors.

Quantum-Based Electronic Devices and Systems

Quantum mechanics, the subfield of physics that describes the behavior of very small (quantum) particles, provides the basis for a new paradigm of computing. First proposed in the 1980s as a way to improve computational modeling of quantum systems, the field of quantum computing has recently garnered significant attention due to progress in building small-scale devices. However, significant technical advances will be required before a large-scale, practical quantum computer can be achieved. Quantum Computing: Progress and Prospects provides an introduction to the field, including the unique characteristics and constraints of the technology, and assesses the feasibility and implications of creating a functional quantum computer capable of addressing real-world problems. This report considers hardware and software requirements, quantum algorithms, drivers of

advances in quantum computing and quantum devices, benchmarks associated with relevant use cases, the time and resources required, and how to assess the probability of success.

Handbook of Optoelectronic Device Modeling and Simulation

An overview of semi-classical gravity theory and stochastic gravity as theories of quantum gravity in curved space-time.

Quantum Computing

Computational methods are rapidly becoming major tools of theoretical, pharmaceutical, materials, and biological chemists. Accordingly, the mathematical models and numerical analysis that underlie these methods have an increasingly important and direct role to play in the progress of many areas of chemistry. This book explores the research interface between computational chemistry and the mathematical sciences. In language that is aimed at non-specialists, it documents some prominent examples of past successful cross-fertilizations between the fields and explores the mathematical research opportunities in a broad cross-section of chemical research frontiers. It also discusses cultural differences between the two fields and makes recommendations for overcoming those differences and generally promoting this interdisciplinary work.

Large-scale Simulations of Error Prone Quantum Computation Devices

Written primarily for advanced undergraduate and masters level students in physics, this text includes a broad range of topics in applied quantum optics such as laser cooling, Bose-Einstein condensation and quantum information processing.

Quantum Chemistry and Dynamics of Excited States

Semiconductor quantum optics is on the verge of moving from the lab to real world applications. When stepping from basic research to new technologies, device engineers will need new simulation tools for the design and optimization of quantum light sources, which combine classical device physics with cavity quantum electrodynamics. This thesis aims to provide a holistic description of single-photon emitting diodes by bridging the gap between microscopic and macroscopic modeling approaches. The central result is a novel hybrid quantum-classical model system that self-consistently couples semi-classical carrier transport theory with open quantum many-body systems. This allows for a comprehensive description of quantum light emitting diodes on multiple scales: It enables the calculation of the quantum optical figures of merit together with the simulation of the spatially resolved current flow in complex, multi-dimensional semiconductor device geometries out of one box. The hybrid system is shown to be consistent with fundamental laws of (non-)equilibrium thermodynamics and is demonstrated by numerical simulations of realistic devices.

Coherent Raman Scattering Microscopy

Opening with a brief historical account of electron transport from Ohm's law through transport in semiconductor nanostructures, this book discusses topics related to electronic quantum transport. The book is written for graduate students and researchers in the field of mesoscopic semiconductors or in semiconductor nanostructures. Highlights include review of the cryogenic scanning probe techniques applied to semiconductor nanostructures.

Quantum Algorithms Via Linear Algebra

This book contains selected papers presented at the First NASA International Conference on Quantum Computing and Quantum Communications, QCQC'98, held in Palm Springs, California, USA in February 1998. As

the record of the first large-scale meeting entirely devoted to quantum computing and communications, this book is a unique survey of the state-of-the-art in the area. The 43 carefully reviewed papers are organized in topical sections on entanglement and quantum algorithms, quantum cryptography, quantum copying and quantum information theory, quantum error correction and fault-tolerant quantum computing, and embodiments of quantum computers.

Electrically Driven Quantum Dot Based Single-Photon Sources