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Applications of nanotechnology continue to fuel significant innovations in areas ranging from electronics, microcomputing, and biotechnology to medicine, consumer supplies, aerospace, and energy production. As progress in nanoscale science and engineering leads to the continued development of advanced

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materials and new devices, improved methods of modeling and simulation are required to achieve a more robust quantitative understanding of matter at the nanoscale. Computational Nanotechnology: Modeling and Applications with MATLAB® provides expert insights into current and emerging methods, opportunities, and challenges associated with the computational techniques involved in nanoscale research. Written by, and for, those working in the interdisciplinary fields that comprise nanotechnology—including engineering, physics, chemistry, biology, and medicine—this book covers a broad spectrum of technical information, research ideas, and practical knowledge. It presents an introduction to computational methods in nanotechnology, including a closer look at the theory and modeling of two important nanoscale systems:

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molecular magnets and semiconductor quantum dots. Topics covered include: Modeling of nanoparticles and complex nano and MEMS systems Theory associated with micromagnetics Surface modeling of thin films Computational techniques used to validate hypotheses that may not be accessible through traditional experimentation Simulation methods for various nanotubes and modeling of carbon nanotube and silicon nanowire transistors In regard to applications of computational nanotechnology in biology, contributors describe tracking of nanoscale structures in cells, effects of various forces on cellular behavior, and use of protein-coated gold nanoparticles to better understand protein-associated nanomaterials. Emphasizing the importance of MATLAB for biological simulations in nanomedicine, this wide-ranging survey of computational nanotechnology concludes by discussing

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future directions in the field, highlighting the importance of the algorithms, modeling software, and computational tools in the development of efficient nanoscale systems.

Computational Finite Element Methods in Nanotechnology demonstrates the capabilities of finite element methods in nanotechnology for a range of fields. Bringing together contributions from researchers around the world, it covers key concepts as well as cutting-edge research and applications to inspire new developments and future interdisciplinary research. In particular, it emphasizes the importance of finite element methods (FEMs) for computational tools in the development of efficient nanoscale systems. The book explores a variety of topics, including: A novel FE-based thermo-electrical-mechanical-coupled

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model to study mechanical stress, temperature, and electric fields in nano- and microelectronics The integration of distributed element, lumped element, and system-level methods for the design, modeling, and simulation of nano- and micro-electromechanical systems (N/MEMS) Challenges in the simulation of nanorobotic systems and macro-dimensions The simulation of structures and processes such as dislocations, growth of epitaxial films, and precipitation Modeling of self-positioning nanostructures, nanocomposites, and carbon nanotubes and their composites Progress in using FEM to analyze the electric field formed in needleless electrospinning How molecular dynamic (MD) simulations can be integrated into the FEM Applications of finite element analysis in nanomaterials and systems used in medicine, dentistry, biotechnology, and

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And Applications With Matlab Nano And Energy other areas The book includes numerous examples and case studies, as well as recent applications of microscale and nanoscale modeling systems with FEMs using COMSOL Multiphysics® and MATLAB®. A one-stop reference for professionals, researchers, and students, this is also an accessible introduction to computational FEMs in nanotechnology for those new to the field.

Positioning itself at the common boundaries of several disciplines, this work provides new perspectives on modern nanoscale problems where fundamental science meets technology and computer modeling. In addition to well-known computational techniques such as finite-difference schemes and Ewald summation, the book presents a new finite-difference calculus of Flexible Local Approximation Methods (FLAME) that qualitatively



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improves the numerical accuracy in a variety of problems.

This reference offers tools for engineers, scientists, biologists, and others working with the computational techniques of nanophotonics. It introduces the key concepts of computational methods in a manner that is easily digestible for newcomers to the field. The book also examines future applications of nanophotonics in the technical industry and covers new developments and interdisciplinary research in engineering, science, and medicine. It provides an overview of the key computational nanophotonics and describes the technologies with an emphasis on how they work and their key benefits.

This book introduces the key concepts of nanoscale spectroscopy methods used in

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nanotechnologies in a manner that is easily digestible for a beginner in the field. It discusses future applications of nanotechnologies in technical industries. It also covers new developments and interdisciplinary research in engineering, science, and medicine. An overview of nanoscale spectroscopy for nanotechnologies, the book describes the technologies with an emphasis on how they work and on their key benefits. It also serves as a reference for veterans in the field.

Computational Modelling of Nanoparticles highlights recent advances in the power and versatility of computational modelling, experimental techniques, and how new progress has opened the door to a more detailed and comprehensive understanding of the world of nanomaterials. Nanoparticles, having

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dimensions of 100 nanometers or less, are increasingly being used in applications in medicine, materials and manufacturing, and energy. Spanning the smallest sub-nanometer nanoclusters to nanocrystals with diameters of 10s of nanometers, this book provides a state-of-the-art overview on how computational modelling can provide, often otherwise unobtainable, insights into nanoparticulate structure and properties. This comprehensive, single resource is ideal for researchers who want to start/improve their nanoparticle modelling efforts, learn what can be (and what cannot) achieved with computational modelling, and understand more clearly the value and details of computational modelling efforts in their area of research. Explores how computational modelling can be successfully applied at the nanoscale level Includes techniques for the computation modelling of different types

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of nanoclusters, including nanoalloy clusters, fullerenes and Ligated and/or solvated nanoclusters Offers complete coverage of the use of computational modelling at the nanoscale, from characterization and processing, to applications

Molecular modeling techniques have been widely used in drug discovery fields for rational drug design and compound screening. Now these techniques are used to model or mimic the behavior of molecules, and help us study formulation at the molecular level. Computational pharmaceutics enables us to understand the mechanism of drug delivery, and to develop new drug delivery systems. The book discusses the modeling of different drug delivery systems, including cyclodextrins, solid dispersions, polymorphism prediction, dendrimer-

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based delivery systems, surfactant-based micelle, polymeric drug delivery systems, liposome, protein/peptide formulations, non-viral gene delivery systems, drug-protein binding, silica nanoparticles, carbon nanotube-based drug delivery systems, diamond nanoparticles and layered double hydroxides (LDHs) drug delivery systems. Although there are a number of existing books about rational drug design with molecular modeling techniques, these techniques still look mysterious and daunting for pharmaceutical scientists. This book fills the gap between pharmaceuticals and molecular modeling, and presents a systematic and overall introduction to computational pharmaceuticals. It covers all introductory, advanced and specialist levels. It provides a totally different perspective to pharmaceutical scientists, and will greatly facilitate the development

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of pharmaceuticals. It also helps computational chemists to look for the important questions in the drug delivery field. This book is included in the Advances in Pharmaceutical Technology book series.

The development of computational methods that support human health and environmental risk assessment of engineered nanomaterials (ENMs) has attracted great interest because the application of these methods enables us to fill existing experimental data gaps. However, considering the high degree of complexity and multifunctionality of ENMs, computational methods originally developed for regular chemicals cannot always be applied explicitly in nanotoxicology. This book discusses the current state of the art and future needs in the development of computational

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modeling techniques for nanotoxicology. It focuses on (i) computational chemistry (quantum mechanics, semi-empirical methods, density functional theory, molecular mechanics, molecular dynamics), (ii) nanochemoinformatic methods (quantitative structure – activity relationship modeling, grouping, read-across), and (iii) nanobioinformatic methods (genomics, transcriptomics, proteomics, metabolomics). It reviews methods of calculating molecular descriptors sufficient to characterize the structure of nanoparticles, specifies recent trends in the validation of computational methods, and discusses ways to cope with the uncertainty of predictions. In addition, it highlights the status quo and further challenges in the application of computational methods in regulation (e.g., REACH, OECD) and in industry for product development and optimization

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And the future directions for increasing acceptance of computational modeling for nanotoxicology.

Illustrates the application of mathematical and computational modeling in a variety of disciplines With an emphasis on the interdisciplinary nature of mathematical and computational modeling, *Mathematical and Computational Modeling: With Applications in the Natural and Social Sciences, Engineering, and the Arts* features chapters written by well-known, international experts in these fields and presents readers with a host of state-of-the-art achievements in the development of mathematical modeling and computational experiment methodology. The book is a valuable guide to the methods, ideas, and tools of applied and computational mathematics as they apply to other disciplines such as the



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natural and social sciences, engineering, and technology. Mathematical and Computational Modeling: With Applications in the Natural and Social Sciences, Engineering, and the Arts also features: Rigorous mathematical procedures and applications as the driving force behind mathematical innovation and discovery Numerous examples from a wide range of disciplines to emphasize the multidisciplinary application and universality of applied mathematics and mathematical modeling Original results on both fundamental theoretical and applied developments in diverse areas of human knowledge Discussions that promote interdisciplinary interactions between mathematicians, scientists, and engineers Mathematical and Computational Modeling: With Applications in the Natural and Social Sciences, Engineering, and the Arts is an ideal resource for

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Computational Engineering. The book also  
serves as an excellent textbook for  
graduate courses in mathematical  
modeling, applied mathematics, numerical  
methods, operations research, and  
optimization.

Understanding the physical properties and dynamical behavior of nanochannel flows has been of great interest in recent years and is important for the theoretical study of fluid dynamics and engineering applications in physics, chemistry, medicine, and electronics. The flows inside nanoscale pores are also important due to their highly beneficial drag and heat transfer properties. Nanoscale Flow:

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presents the latest research in the multidisciplinary area of nanoscale flow.

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this comprehensive book: Highlights the current status of research on nucleate pool boiling heat transfer, flow boiling heat transfer, and critical heat flux (CHF)

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Explores thermal conductivity enhancement in nanofluids measured with a hot-wire calorimeter Discusses two-phase laminar mixed convection  $Al_2O_3$  water nanofluid in an elliptic duct

Explains the principles of molecular and omics imaging and spectroscopy techniques for cancer detection Analyzes fluid dynamics

modeling of the tumor vasculature and

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drug transport Studies the properties of nanoscale particles and their impact on diagnosis, therapeutics, and theranostics Provides a brief background and review of medical nanoscale flow applications Contains useful appendices of physical constants, equations, common symbols, mathematical formulas, the periodic table, and more A valuable reference for engineers, scientists, and biologists, Nanoscale Flow: Advances, Modeling, and Applications is also designed for researchers, universities, industrial institutions, and government, giving it broad appeal.

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