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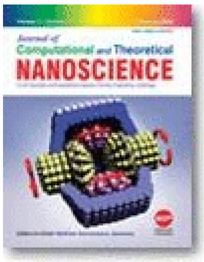

Modelling Coupled and Transport Phenomena in Nanotechnology

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This special issue contains refereed papers based on invited presentations at the special session on "Modeling Coupled and Transport Phenomena in Nanotechnology" of the Third M.I.T. Conference on Computational Fluid and Solid Mechanics, June 14 - 17, 2005.

Guest Editorial: Special Issue of the Journal of Computational and Theoretical Nanoscience on Modelling Coupled and Transport Phenomena

Many nanoscale phenomena can be understood better by using tools of mathematical modelling and computational experiment applied at the interface of atomistic and molecular modeling and continuous solid and fluid mechanics. The forces of different range and scale are present in nanoscale phenomena including inter-atomic, magnetic, and electrical. Stress-induced and thermal effects may influence the properties of nanostructures and are often of fundamental importance in describing many phenomena at the nanoscale level. The numerical algorithms that are capable of handling these coupled phenomena and the physical description of nano- and microscale phenomena obtained with such numerical algorithms are rapidly becoming an indispensable tool in the development of nanoscience and its applications.

Motion of submicron charged particles in nanoscale self-assembly processes, motion of feedstock gas in production of carbon nanotubes (CN), and carrier dynamics in semiconductor heterostructures applied in electronic industry are important examples of coupled and transport phenomena at the nanoscale level. The effect of such coupled and transport phenomena on the properties of nanomaterials and nano/micro-structures was one of the major topics of the workshop on Modelling Coupled and Transport Phenomena in Nanotechnology that took place within the Third M.I.T. Conference on Computational Fluid and Solid Mechanics in Cambridge, Massachusetts.

The tendency of ultra-large scale integration of electronic components will continue into the future, requiring new models and tools to be developed. In this context, several workshop contributions discussed non-local mathematical models that are able to describe non-equilibrium transport of semiconductor plasma. New models and algorithms in quantum semiconductor physics that play a fundamental role in many nanotechnological applications were discussed. Our focus in this context was on the modelling of semiconductor superlattices and low-dimensional semiconductor systems such as quantum dots, wires, and rods, and the description of their opto-electromechanical properties. Due to atomistic discontinuities at interfaces between different materials it is possible to take advantage of confined nanoscale quantum states in such structures. Several contributions in this special issue address challenges associated with the modelling of such structures and their applications.

Another group of contributions to this special issue deals with transport phenomena. Transport phenomena are especially important for technological applications and continuous production, handling, and use of nano-materials. The majority of applied nano-scale processes occurs in the presence of fluid (liquid, gas, plasma, or multi-phase flow) that may function as a carrier of particles transported through micro- or nano- scale pores and channels, feedstock of carbon in synthesis of nanotubes, and a heating or cooling agent. The fluid motion defines the temperature of catalyst particles and the local chemical composition of the fluid that determines the success of nanotube synthesis. Several contributions to this issue discuss the multi-model approach for concurrent rendering of different areas of computational domain by different models and/or different time steps for the same model including a strong mutual relation between models at different scales. For example, in multiple plume ejection in the laser ablation method for production of nanotubes, the ablation of carbon occurs in 10-20 nanoseconds whereas the synthesis of nanotubes occurs in the micro- to milli-second scale range. Despite the nano-scale nature of the phenomena dealt with in this group of contributions, it is unnecessary and unrealistic to resolve the entire flow-field in the nano-meter scale of spatial resolution. Instead, several approaches discussed in this issue deal with the continuous mechanics of flow with partial slip boundary conditions reflecting molecular dynamics near the rigid wall, a micro-fluidic flow model that is needed to describe the fluid flow about fibers, and the stability analysis of micro- and nano- fluids. Contributions on other important tools of mathematical modelling applied to the analysis of nano- and micro-scale phenomena such as boundary elements method and the lattice Boltzmann approach are also presented.

Each contribution to this special issue of the Journal of Computational and Theoretical Nanoscience has been selected on the basis of a peer-reviewed process. We thank the authors for their contributions, the referees of this special issue for their time, their efforts, and their helpful suggestions, and Dr Wolfram Schommers for his support.

We hope that this special issue of the Journal of Computational and Theoretical Nanoscience on Modelling Coupled and Transport Phenomena will stimulate further progress in this important area via interdisciplinary efforts of physicists, engineers, mathematical modellers, and chemists.

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