

Computational Nanotechnology: A Current Perspective

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Abstract: The current status of the progress and developments in *computational nanotechnology* is briefly reviewed, from the perspective of its applications. The enabling tools and techniques of physics- and chemistry-based simulations, within a multi-scale context, are briefly reviewed.

1 Introduction

Nanotechnology deals with materials, devices, and their applications, in areas such as engineered materials, electronics, computers, sensors, actuators, and machines, at the nano length-scale. Atoms and molecules, or extended atomic or molecular structures, are considered to be the basic units, or building-blocks, of fabricating future generations of electronic devices, and materials. At the nano-meter length scales, many diverse enabling disciplines and associated technologies start to merge, because these are derived from the rather similar properties of the atomic- or molecular- level building blocks. For example, on the one hand, the DNA molecular strands are these days proposed as the self-assembling templates for bio-sensors and detectors, molecular electronics, and as the building blocks of all biological materials. On the other hand, some synthetic inorganic materials, such as carbon, boron-nitride or other nanotubes or nanowires, may also have similar functionalities in some respects, but could also be exceptionally strong and stiff materials. The cross-correlation and fertilization among the many constituent disciplines, as enabling technologies for molecular nanotechnology, are thus essential for an accelerated development.

In the simplest terms, the subject of nanoscience/technology is defined as the science and

technology of the direct or indirect manipulation of atoms and molecules into functional structures, with applications that were never envisioned before. The prefix “nano” corresponds to a basic unit on a length scale, meaning 10^{-9} meters, which is a hundred to a thousand times smaller than a typical biological cell or bacterium. At the nanometer length scale, the dimensions of the materials and devices, begin to reach the limit of 10 to 100s of atoms, wherein entirely new physical and chemical effects are observed; and possibilities arise for the next generation of cutting-edge products based on the ultimate miniaturization or so called “nanoization” of the technology. The earliest impetus to the scientific and technological possibility of coaxing individual atoms into the making of useful materials, devices and applications was given by the late Nobel- prize winning physicist Richard Feynman, in a land mark lecture: “There’s Plenty of Room at the Bottom,” delivered at the American Physical Society (APS) meeting at Cal Tech in 1959, in which he said, “*The problems of chemistry and biology can be greatly helped if our ability to see what we are doing, and to do things on an atomic level, is ultimately developed - a development which I think cannot be avoided.*” Indeed, scanning probe microscopes (SPMs), in recent years, have already given us this ability in limited domains, and spurred a tremendous growth in the pursuit of nanotechnology in the last two decades. A series of scientific and technological discoveries and progresses in a variety of areas in 1970s and 1980s, and the enunciation of visionary scenarios by Eric Drexler in a possible molecular nanotechnology-enabled world, have revived the field in the 1980-90s.

The real progress in the last decade, has been due to a series of advances in a variety of complementary areas, such as: the discoveries of atomically precise materials such as nanotubes and fullerenes; the ability of the scanning probe and the development of manipulation techniques to image and manipulate atomic and molecular configurations in real materials; the conceptualisation and demonstration of individual electronic and logic de-

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vices with atomic or molecular level materials; the advances in the self-assembly of materials to be able to put together larger functional or integrated systems; and above all, the advances in *computational nanotechnology*, i.e., *physics- and chemistry- based modelling and simulation of possible nanomaterials, devices and applications*. It turns out that at the nanoscale, devices and systems sizes have shrunk sufficiently small, so that, it is possible to describe their behaviour fairly accurately. The simulation technologies have become also *predictive* in nature, and many *novel* concepts and designs have been *first proposed based on modelling and simulations*, and then were followed by their realization or verification through experiments.

In this brief narrative, we summarize the physics- and chemistry- based methods, which form the foundations of *computational nanotechnology*, and the areas of its possible application, however, in the limited context of the papers covered in this special issue.

2 Computational Nanotechnology: Techniques

The role of *computational nanomechanics* has become critically important in the cycle of growth and development of nanotechnology, because, as mentioned above, the length and time scales of important nanoscale systems and phenomenon have shrunk to the level, where they can be directly addressed, with high-fidelity computer simulations and theoretical modeling. The accuracies in the atomistic and quantum-mechanical methods have increased to the level, whereby simulations have become truly predictive in nature. The CPU cycles available for simulations and the emergence of 3d visualization tools and large data manipulation/mining packages have contributed significantly to the growth of computational nanotechnology in recent years. Computational nanotechnology is emerging as a fundamental engineering analysis tool for the novel designs of nanodevices, much in the same way as the continuum finite element analysis (FEA) has been used for the design and analysis of most of the current generation of engineering systems (e.g., automobiles, ships, airplanes, MEMS devices, and ICs).

From the computer-simulation perspective, the problem is truly multiple length-&-time-scale in nature. For example, the region of interest for direct simulations, extends from the basic atomistic sub-nanometer length scale, to the 10-100s of nanometers in the intermediate

range, and then on to the truly micron or larger size materials, devices and systems. At the atomistic level, there are accurate semi-classical and quantum molecular mechanics methods, that feed into the large scale classical MD simulations with 10s of millions to few billions of atoms, which then could be coupled to mesoscopic (micron size) devices and systems described through continuum mechanics or finite element based approaches. Initial attempts have been made to develop a “grand-simulation code or tool” cutting across different length scale and achieving a seamless integration across the interfaces (Nakano et. al., 1997, Rudd et. al.,). Similar approaches to bridge phenomenon along the time axis have been attempted through multiple-time scale simulations in a single system, but most of these work for specific applications, but do not work otherwise. Current attempts at a seamless simulation of multiple-length-scales phenomena are also based on the Meshless Local Petrov Galerkin Methods, using moving least squares interpolations [Atluri and Shen (2002a,b)]. In the last few years, attempts, however, have also been made on attacking the “right” type of problem with an appropriate “right” type of simulation tool [Srivastava et. al., (2001)] across a wide range of applications.

In this section, we briefly summarize the main simulation approaches, spanning across mainly the different length scales.

Starting from the bottom-up, a few 10s to hundreds of atoms are very accurately simulated with the *ab initio* (or first principles) quantum mechanical methods, wherein simulations are aimed towards the solution of the complex quantum many-body Schroedinger equation of the atomic system (including nuclei and electrons), using numerical algorithms (Payne et. al, 1992). *Ab-initio* methods provide more accurate descriptions of quantum mechanical behavior of materials, even though the system sizes currently are limited to only about a few hundred atoms. Current *ab-initio* simulation methods in condensed phase materials, clusters, nanotubes and wires are based on a rigorous mathematical foundation of the density functional theory (DFT) (Hohenberg et. al., 1964). This is derived from the fact that the ground-state total electronic energy is a functional of the density of the system. For practical applications, the DFT-LDA method has been implemented, with a pseudopotential approximation and a plane wave (PW) basis expansion of single electron wave functions (Payne et.

al., 1992). These approximations reduce the electronic-structure problem to a self-consistent matrix diagonalization problem. At the end of the iterative matrix diagonalization procedure, the resulting eigen-values correspond to the quantum-mechanically possible electronic energy states of the system, and eigen-functions contain information about the electronic density distribution in the computed space. One of the popular DFT simulation programs is the Vienna Ab initio Simulation Package (VASP), which is available through a license agreement (Hafner, 1999). In this regime, there are also the quantum-chemistry based methods, which are generally more suitable to molecular systems of smaller size, but the advantage is that, the electronically excited states can be accommodated in these methods. The applications in opto-electronics, quantum computations or quantum information processing, need the transitions among the excited states, that are not covered in the above mentioned DFT based simulation techniques.

Coupled with the electronic-structure solution of the many atoms system, is also the possibility of simulating the dynamic evolution as a function of time. Several accurate quantum molecular dynamics schemes have been developed, in which the forces between atoms are computed at each time step, via quantum mechanical calculations within the Born-Oppenheimer approximation. The dynamic motion for ionic positions are still governed by the Newtonian or Hamiltonian mechanics, and described by molecular dynamics. The most widely known and accurate scheme is the Car-Parrinello (CP) molecular dynamic method [Car-Parrinello, 1985], wherein the electronic states and atomic forces are described using the *ab-initio* DFT method.

In the intermediate regime of a few hundred- to thousand-atom systems, tight-binding [Harrison, 1980], or semi-empirical quantum mechanics based methods, provide an important bridge between the *ab-initio* quantum mechanics based approaches described above, and the classical atomistic force field based methods, that will be described below. The computational efficiencies of the tight-binding or semi-empirical methods derive from the fact, that the quantum Hamiltonian of the system can be parameterized. Furthermore, the electronic-structure information can also be easily extracted from the tight-binding Hamiltonian, which also contains the effects of angular inter-atomic forces in a natural way. The tight-binding structure and molecular dynamics methods have

been parametrized for a variety of molecular and materials systems. For structural problems, diagonalization of large matrices are needed only a few times, and hence relatively large systems (up to 100,000s of atoms) have been simulated with order-N tight-binding methods, implemented on parallel computers. For dynamic problems, non-orthogonal tight-binding molecular dynamics schemes are more accurate, but are not easily converted to order N type, and can typically handle only systems with up to a few thousand atoms [Menon et. al., 1997].

For larger systems (million to billion atoms), the classical molecular dynamics (MD) simulations, which refer most commonly to the situation wherein the motion of atoms or molecules is treated in approximate finite difference equations of Newtonian mechanics. Except when dealing with very light atoms and very low temperatures, the use of classical mechanics is well justified. The dynamics of complex condensed phase systems, such as metals and semiconductors, is described with explicit or implicit many-body force field functions, using the Embedded Atom Method (EAM) type potentials for metals, and Stillinger-Weber (SW) and/or Tersoff-Brenner (T-B) type potentials for semiconductors (Garrison et. al., 1996). The Tersoff-Brenner type potentials (Brenner et. al., 1998) are parameterized for, and specially are suited for, carbon based systems, such as carbon nanotubes, and have been used in a wide variety of scenarios, with the obtained results being in agreement with some of the experimental observations. However, currently, there is no universal classical force field function, which works for all the materials and in all the scenarios. Consequently, one needs to be careful, especially where true chemical changes (involving electronic rearrangements) with large atomic displacements are expected to occur.

In its global structure, a general MD method typically implements an algorithm to find a numerical solution of a set of coupled first-order ordinary differential equations, given by the Hamiltonian formulation of Newton's Second Law. The equations of motion are numerically integrated forward, in finite time steps. For reactive force field functions, chemical bonds can form and break during the course of a simulation. Therefore, as compared to some other molecular dynamics methods, the neighbor-list describing the environment of each atom includes only a few atoms and needs to be updated more frequently. Most of the commercial molecular dynamics codes, geared towards bio-molecular simulations,

use non-reactive force field functions which are good for structure and conformation optimization purposes, and in the situations where no reactions occur during the dynamics. The computational cost of the many-body bonded interactions is relatively high, as compared to the cost of similar methods with non-reactive interactions with simpler functional form. Efficient parallel codes have been developed to handle solutions of millions to billion of coupled first order differential equations with strategies depending on the nature of inter atomic force field functions. [Srivastava et. al. (2001) and Nakano et. al. 2001]. Recent attempts are also made, using the Meshless Local Petrov Galerkin (MLPG) Method, and the moving least-squares interpolations [Atluri & Shen (2002a,b)] to specify and control the neighborhood of each atom.

The static and dynamic structural simulations of nanoscale systems, are only a part of a range of simulations needed, to carry the simulated systems to the level of applications. The remaining part is obviously the mechanical, chemical, and electronic characterization, that also comes through the intelligent use of the above described techniques, as well as the dynamic-response simulations to find the thermal, electrical and magnetic response under external fields. Detailed characterizations of the system, under these conditions, are needed for exploring the applications in nanoscale electronic, electromechanical, opto-electronic and magnetic device systems.

The technology-development at the nanoscale can be driven and guided, to a large extent, by the theoretical modeling and the state-of-the-art simulations, because of the predictive capabilities of these techniques, and their ability to characterize many systems at a much faster rate. As an example, carbon nanotubes have been proposed for a variety of applications in electronics, computing, structural materials, sensors, and molecular machines. Most of the proposed applications have come out the theoretical modeling and simulation studies, which predicted: (a) high electronic and thermal conductivities of carbon nanotubes, (b) nanotube junctions for electronic devices, and (c) nanotubes as reinforcing fibers in light-weight, high-strength composite materials (Srivastava et. al., 2001). The pace of the computer-simulation work has, thus, kept at par or some times even been ahead of the experimental work. For example, branched nanotube junctions shown in Fig.1, were first proposed as components of molecu-

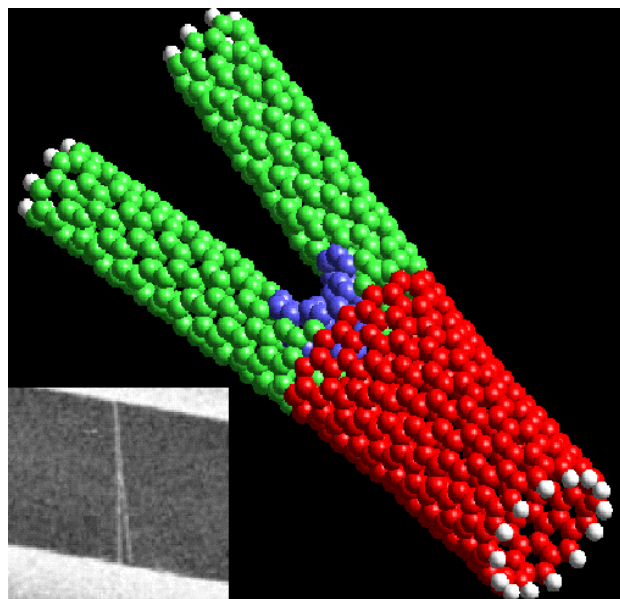


Figure 1 : Model of a single-wall carbon nanotube Y-junction first predicted in simulation based studies and inset shows a multi-wall carbon nanotube Y-junction fabricated in experiments and shown to work as an electronic device.

lar electronic devices, through modeling and simulation studies (Menon et. al. (1997, 1998)), but were fabricated (multiwall-nanotube Y junctions) only recently, in many experiments with much control and different pathways (Papadopolous et. al. (2000) and Satishkumar et. al, (2000)). The simulations have also showed their use as analog logic devices, and recent experiments have observed similar current-voltage characteristics under similar conditions (Andriotis et. al., (2002)). Very recent experiments have even shown the possibility of creating junctions of single-wall nanotubes, by e-beam induced welding of two nanotubes in contact (Terrones et. al., (2002)). As the capabilities for computing and simulation increase, and algorithms and implementations are refined, many more such areas and examples will occur, wherein, the simulation based rapid-prototyping of the yet to be fabricated nanoscale systems will be a norm and not an exception.

3 Computational Nanotechnology: Applications

This special issue of *Computer Modeling in Engineering and Sciences* is devoted to a collection of technical papers with a common theme of dealing with various

aspects of nanotechnology. Nanotechnology is a truly a multidisciplinary field, spanning across many core physical sciences and engineering areas. The role of computational nanotechnology as the enabling technology, for conceptualisation, characterization, development and prototyping of nanoscale materials, devices and systems applications, is vast and beyond the scope of being fully covered in a single issue. However, an attempt has been made to expose readers to the paradigm of how *computational nanotechnology* can be used to not only understand and characterize the systems under experimental investigation, but also as to how predictions can be made for novel applications, because there is a strong coupling between the structural, mechanical, chemical and electronic properties at the nano-scale.

A comprehensive paper by Brenner et al (Brenner et. Al. 2002) covers the details of physics- and chemistry-based many-body atomistic and self-consistent tight-binding simulation methods, and applies it to a very broad range of applications in carbon based materials and devices. The paper shows that it is indeed possible to develop hierarchical simulation techniques with applicability depending on what the system size is, and what level of accuracy is needed. The structure and molecular dynamics (MD) are based on Brenner's own many-body bond-order reactive potential, developed and refined through the 1990s, and the electronic effects are included through the traditional tight-binding and a newly developed self-consistent tight-binding methods. The self-consistent tight-binding is shown to incorporate a description of the charge transfer as well. The applications to a wide variety of carbon based materials and devices are covered. The examples are the functionalised and kinked carbon nanotubes for nanoelectronic and sensor applications, hydrogen storage in carbon nanotubes as gas transportation devices, nanotubes in polymer composites for structural reinforcement in light-weight high-strength materials, nanotribology at the interface of nanotubes and graphite to understand atomic level details of friction at nanoscale, characterization of nanotubes for field emission, and carbon nanocones, nanorods, and penta-particles for yet a new class of structures that have not been as much investigated as the carbon nanotubes and fullerenes.

The paper by Sinnott et. al., (Sinnott et. al., (2002)) describes the molecular dynamics simulations of the diffusion of gases through carbon-nanotube based membranes, for filtering applications. Zeolites and other nat-

urally occurring nano-porous materials have been traditionally used for gas separation and filtration applications. Carbon-nanotube based membranes could provide a mechanism to synthesize such materials for controllable gas separation applications. The results are useful, in that they indicate that nanotubes may function well as molecular sieves, and thus may be useful as selective membranes. It is interesting that both the insides of the tubes and the interstitial spaces can function in this manner. The systems examined include gaseous sample with small organic molecules and carbon-dioxide. At thermal velocities molecules are found to diffuse from areas of high density to low density through nanotubes or through interstitial pores in a nanotube bundle. The diffusion and separation of molecular mixture strongly depends on the relative sizes of the nanotube and the molecular species in the gaseous mixture.

Applications of carbon nanotubes in the field emission type devices and nano-electromechanical sensors are covered in detail in the paper by Maiti. (Maiti, (2002)). The reported simulations are based on First Principles Density Functional Theory (DFT), classical molecular mechanics, and tight-binding transport based on the recursive Green's function formalism. An interesting use has been made of the structure-optimization for larger systems through classical molecular mechanics based simulations, and then performing the more accurate DFT and tight-binding transport calculations on smaller pieces to connect to experimental observations relevant to applications. The effect of the gaseous adsorbate such as H, on the field emission property of a carbon nanotube tip, is described, and is expected to play a role in the degradation of the material for field emission application in ambient conditions over long time. The nano-electromechanical sensor applications are discussed, through the simulations of AFM tip induced deformation, in a carbon nanotube stretched across two electrodes. Recent experimental measurements have shown that current-voltage characteristics are highly sensitive to such deformations and simulations have attempted to explain the experimental observations with large changes in the conductivity as a function of localized tip-deformed bending of the nanotube.

The paper by Yang et. al., (Yang et. al. (2002)) also deals with a similar objective, i.e., the possible use of carbon nanotubes in nano-electromechanical devices. In nanoscale covalent materials and systems, the coupling

between the electronic properties and mechanical deformations is rather strong. From the very beginning, therefore, applications have been envisioned, wherein the mechanical deformations in a nanotube could cause large changes in the current flowing through the nanotube. This could be used for nano-electromechanical sensor or actuator applications. Based on the simple deformation of the underlying graphene lattice, Yang et al., have been able to construct an analytical model of the correlation between the mechanical deformation of nanotubes and the resulting changes in the electrical conductivity of the deformed nanotube. The model has been supported with simulations of electrical conductivity of axially and torsionally deformed nanotubes, for small and large strain, within a 4-orbital tight-binding description of the electronic Hamiltonian. The authors conclude that their 4-orbital tight-binding results are similar to their earlier work using a pi electron description of nanotubes, and also are in agreement with the general prediction of the analytical model.

Taking a break from the computational nanotechnology of carbon nanotube based devices and applications, the paper from Zhigilei et. al., (Zhigilei et. al. (2002)) is an example of the development of a multi-scale model of the simulation of laser ablation and cluster deposition of nanostructured materials, for system sizes extending from atomistic to meso-scale length scale. The method is developed, for the laser coupling of organic materials and metals, with the initial stages of laser ablation simulated with atomistic MD method. For the mesoscale length regimes, a combined MD - finite element method, and the dynamic boundary condition, are used to avoid a reflection of the laser-induced pressure wave from the boundary of the MD computational cell. A direct simulation Monte Carlo method is then used for the simulation of the long term ablation plume expansion, and the MD method is used to simulate the film growth by nano-scale cluster deposition from the ablation plume.

The paper by Klimeck et. al., (Klimeck et. al. (2002)) is a comprehensive description of a 3-D nanoelectronic simulator tool, suitable for electronic structure and transport in nanoscale devices, including the quantum effects and non-homogenous description of atomic structure and strain distribution. The paper describes a coherent methodology, within a tight-binding framework, for truly 3-D structures with multi-million atoms in the simulation. Specific numerical, algorithmic and compu-

tational advances have been achieved through the implementation of a custom parallel matrix solver, and with applications to the electronic structure and strain distribution in embedded $\text{In}_x\text{Ga}_{(1-x)}\text{Al}$ quantum dots in solid-state materials. It has been possible to include a realistic description of disorder in the alloy, which leads to differences in the energy levels of several meV. These realistic numbers are possible, because calculations are performed on multi-million atom quantum dots, and the developed tool may have future applications in the description of electronic structure and transport in other nanoscale materials, such as carbon nanotubes and DNA, as well.

Lastly, in this issue, the paper by Globus et. al., (Globus et. al. (2002)) is an attempt to develop the an enabling tool and technology, for extending the reactive molecular dynamics simulations to non-carbon based materials and systems as well. So far such simulations have been limited to Si, Ge, and a few other hydrocarbon based systems, because the underlying reactive force field functions for materials containing other atomic species simply do not exist. Developing the reactive multi-atomic force field functions for new systems is difficult and tedious. There are two parts to such a development: first the conceptualization of a physics-based functional form for inter-atomic interactions, and second, the fitting of parameters in a complex many-dimensional space to reflect the correct physical and chemical properties. A genetic-algorithm based procedure, implemented in Java on a cycle scavenging system, has been developed and described for fitting the parameters in a complex many-dimensional function. As an example, the procedure has been applied to fitting the parameters for a Si potential based on the well known Stillinger-Weber functional form. The procedure not only reproduces parameters of the published S-W potential, but also fits a new set of parameters that give better energies of small and large size Si clusters, which were not used in the fitting procedure. The method is promising and could become an important tool in developing reactive force field functions for the molecular dynamics of the systems containing other atomic species in future.

In summary, the future of computational nanotechnology is bright, and strongly correlated with the growth and developments in nanotechnology. A brief review of the current status and examples of the applications covered in this special issue shows that large scale modeling and

simulation will not only play a critical role in the gradual advances, but also may some day yield revolutionary concepts for the novel technologies in a wide variety of nanotechnology related areas. Concepts and applications for novel nanomaterials, electronics, sensing, filtration, laser-processing, and enabling technologies are covered in this special issue. Other contributing growth areas, within the overall spectrum of nanotechnology, related to bio-nanotechnology and healthcare sectors such as bio-informatics, protein folding, nanoscale mechanisms of drug delivery are certainly missing from the simulation and modeling perspective. In the future, this would be remedied by special issues of this journal, focused on these specialized applications.

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References

- Atluri S.N.; and Shen S.** (2002): *The Meshless Local Petrov-Galerkin (MLPG) Method*, 440 pages, Tech Science Press.
- Atluri S.N.; Shen S.P.** (2002): The meshless local Petrov-Galerkin (MLPG) method: A simple & less-costly alternative to the finite element and boundary element methods, *CMES-Computer Modeling in Engineering & Sciences*, 3 (1): 11-51.
- Brenner D. W; Sherendova O. A; Areshkin A** (1998): Quantum Based Analytic Interatomic Forces and Materials Simulations, *Reviews in Computational Chemistry*, VCH Publishers, New York, 213-245.
- Brenner D. W; Shenderova O. A.; Areshkin A., Schall J. D. and Frankland S. J. V** (2002): Atomic Modeling of Carbon-Based Nanostructures as a Tool for Developing New Materials and Technologies, *CMES-Computer Modeling in Engineering & Sciences* Vol. 3, no. 5, 643-673.
- Car R.; Parrinello M.** (1985): Unified Approach for Molecular Dynamics and Density Functional Theory, *Phys. Rev. Lett.* Vol. 55, 2471-2474.
- Garrison B. J.; Srivastava D.** (1995): Potential Energy Surfaces for Chemical Reactions at Solid Surfaces, *Ann. Rev. Physical Chemistry*, Vol. 46, 373.
- Globus A.; Menon M.; Srivastava D.** (2002): Jav-aGenes: Evolving Molecular Force Field Parameters with Genetic Algorithm, *CMES-Computer Modeling in Engineering & Sciences* Vol. 3, no. 5, 557-574.
- Hohenberg P.; Kohn W.** (1964): Inhomogenous Electron Gas, *Phys. Rev. Vol.* 136, B864-B871.
- Hafner J.** (1999): *VAMP/VASP Guide*, <http://cms.mpi.univie.ac.at/vasp> (current 5 June 2001)
- Harrison W. A.** (1980): *Electronic Structure and Properties of Solids*, W. H. Freeman, San Francisco.
- Klimeck G.; Oyafuso F.; Boykin T. B.; Bowen C. R.; Allmen P v** (2002): Development of a Nanoelectronic 3-D (NEMO-3D) Simulator for Multimillion Atom Simulations and its Applications to Alloy Quantum Dots, *CMES-Computer Modeling in Engineering & Sciences* Vol. 3, no. 5, 601-642.
- Maiti A** (2002): Select Applications of Carbon Nanotubes: Field Emission Devices and Electromechanical Sensors, *CMES-Computer Modeling in Engineering & Sciences* Vol. 3, no. 5, 589-599.
- Menon M.; Subbaswami K. R.** (1997): Non-Orthogonal Tight-binding Scheme for Silicon with Improved Transferability, *Phys. Rev. B.* Vol. 55, 9231-9234.
- Menon M.; Srivastava D.** (1997): Carbon Nanotube T-junctions: Nanoscale Metal-Semiconductor-Metal Contact Devices, *Phys. Rev. Lett.* Vol. 79, 4453-4456.
- Menon M.; Srivastava D.** (1998): Carbon Nanotube based Molecular Electronic Devices, *J. Mat. Research*, Vol. 13, 2357.
- Nakano A.; Bachlechner M. E.; Kalia R. K.; Lidorikis E.; Vashishta P.; Campbell T. J.; Ogata S.; Shimojo F.** (2001): Multiscale Simulations of Nanosystems, *Computers in Engineering and Sciences*, Vol. 3, 56-66.
- Papadopoulos C et. al.** (2000): Electronic Transport in Y Junction Carbon Nanotubes, *Phys. Rev. Lett.* Vol. 85, 3476-79.
- Payne M et. al.** (1992): Iterative Minimization Techniques for Ab-Initio Total Energy Calculations: Molecular Dynamics and Conjugate Gradients, *Rev. Mod. Physics*, Vol. 68, 1045-1097.
- Rudd R. E.; Broughton J. Q.** (2000): Coherent Coupling of Length Scales in Solid State Systems, *Physica Status Solidi B*, Vol. 217, 251-291.
- Satishkumar C et. al.** (2000): Y-junction Carbon Nanotubes, *Appl. Phys. Lett.* Vol. 77, 2530-2532.

Srivastava D.; Menon M.; Cho K. (2001): Computational Nanotechnology with Carbon Nanotubes and Fullerenes, *Computing in Engineering and Sciences*. Vol. 3, 42-55.

Sinnott S. B.; Mao Z.; Lee K-H (2002): Computational Studies of Molecular Diffusion Through Carbon Nanotube Membranes, *CMES-Computer Modeling in Engineering & Sciences* Vol. 3, no. 5, 575-587.

Terrones M.; Banhart F.; Grobert N.; Charlier J-C; Terrones H.; Ajayan P. M. (2002): Molecular Junctions by Joining Single-wall Carbon Nanotubes, *Phys. Rev. Lett.* Vol 89, 75505-75508.

Yang L.; Han J., Anantram M. P.; Richard J (2002): Bonding Geometry and Bandgap Changes of Carbon Nanotubes Under Uniaxial and Torsional Strain, *CMES-Computer Modeling in Engineering & Sciences* Vol. 3, no. 5, 675-685.

Zhigilei L. V.; Dongare A. (2002): Multiscale Modeling of Laser Ablation: Applications to Nanotechnology *CMES-Computer Modeling in Engineering & Sciences* Vol. 3, no. 5, 539-555.