

COMPUTATIONAL NANOTECHNOLOGY WITH CARBON NANOTUBES AND FULLERENES

The authors envision computational nanotechnology's role in developing the next generation of multifunctional materials and molecular-scale electronic and computing devices, sensors, actuators, and machines. They briefly review computational techniques and provide a few recent examples derived from computer simulations of carbon nanotube-based molecular nanotechnology.

During the second half of the 20th century, a microelectronics revolution moved us from vacuum tube electronic computers to silicon-based integrated electronic devices. As the 21st century begins, this revolution of scaling, which has traditionally followed Moore's law, is facing major obstacles. To move forward, the science and technology community is tentatively moving from microdevice technology to the emerging field widely known as *nanotechnology*.

The science and technology of nanoscale materials, devices, and applications in areas such as computers, sensors, actuators, and machines fall within the realm of nanotechnology. For the purposes of this article, we consider atoms and molecules (or extended atomic or molecular struc-

tures) to be the basic units or building blocks of fabricating future generations of electronics, materials, devices, and applications. At nanometer-length scales, many diverse fields and their associated technologies start to merge because the material properties are derived from the molecular building blocks. The molecularly perfect structure that produces exceptionally strong structural and mechanical behavior in one class of system applications can also produce the exotic electronic and chemical behavior in another class.

The role of *computational* nanotechnology has become critically important in nanotechnology development. The length and time scales of nanoscale systems and phenomenon have shrunk to where we can directly address them with computer simulations and theoretical modeling with high accuracy. The rapidly increasing computing power used for large-scale and high-fidelity simulations make it increasingly possible for nanoscale simulations to be also predictive. Computational nanotechnology is emerging as a fundamental engineering analysis tool for novel nanodevice design in the way that continuum finite-element analysis has been used for designing and analyzing most engineering systems.

This article's main objective is to introduce the possibilities of computational nanotechnol-

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otube is obtained. We can connect nanotubes with different chiralities to create nanotube heterojunctions; these junctions form a variety of nanoscale molecular electronic device components.

- SWNTs and MWNTs have good elastomechanical properties because the 2D arrangement of carbon atoms in a graphene lattice allows large out-of-plane distortions, while the strength of carbon-carbon in-plane bonds keeps the graphene sheet exceptionally strong against any in-plane fracture or distortion. All distortions induced in a simulation or observed in a static snapshot of an experiment appear to indicate high elasticity of the nanotubes and point toward their possible use as a lightweight, highly elastic, strong fibrous material.
- Because nanotubes are hollow, tubular, caged molecules, they can act as lightweight, large-surface-area packing material for gas storage and hydrocarbon fuel storage devices, as well as nanoscale containers for molecular drug delivery and casting structures for making nanowires and nanocapsulates.

These three qualities suggest a variety of possible applications. The nanotube heterojunctions with electronic switching properties could influence the next generation of computer component development. Nanotubes with exceptionally stiff and strong mechanical properties can help us make lightweight structural components. Nanotubes as capsules can help us store and carry hydrogen and other hydrocarbon-based fuel in automobiles or aboard spacecraft.

Carbon-based materials are ideally suitable as molecular-level building blocks for nanoscale system design, fabrication, and applications. From a structural or functional materials perspective, carbon is the only element that exists in a variety of shapes and forms with varying physical and chemical properties. All basic shapes and forms needed to build any complex molecular-scale architecture are already available with carbon.

Computational techniques for nanoscale simulations

Until about 40 years ago, researchers computed the thermodynamic properties of interacting, bulk condensed-matter systems with analytical approximation methods for an infinite system. These analytical methods were valid only in the weakly interacting system limit—the approximations still

had to be carried out numerically beyond a few orders. Since then, a new kind of approximation scheme—exact numerical computation of the properties of a finite-sample system—has become the most common approach to studying interacting condensed-matter systems. Molecular dynamics (MD) refers most commonly to the situation where 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.

Until about 20 years ago, MD computations primarily used simplistic pair potentials to describe inert gases in condensed-phase systems or the materials that tend to form hexagonal closed packing structures. A slow transition to describe dynamics of more complex condensed-phase systems such as metals and semiconductors with explicit or implicit many-body force-field functions began with embedded-atom-method type potentials for metals and bond-order type potentials for semiconductors.² Based on the variations of these three types of potentials, researchers have proposed and used a wide variety of force-field functions in classical MD simulations. Many of the potentials are expected to work well in the regimes of physical parameters in which they were constructed in the first place.

However, no universal classical force-field function works for all materials in all scenarios. So, we need to watch for the description of dynamics or reactions with surfaces and clusters where we expect true chemical changes (involving electronic rearrangements) with large atomic displacements.

In recent years, several accurate quantum MD schemes have computed the forces between atoms at each time step with quantum mechanical calculations within the Born-Oppenheimer approximation. The dynamic motion for ionic positions are still governed by Newtonian or Hamiltonian mechanics and described by MD. The most widely known and accurate scheme is the Car-Parrinello MD method,³ which describes the electronic states and atomic forces using the ab initio density functional method (usually within the local density approximation). Although we can now perform such ab initio MD simulations for systems consisting of a few hundred atoms, for a vast range of system sizes such calculations start to stretch the limits of present-day computational resources. In the intermediate regimes between large-scale classical MD and quantum Car-Parrinello MD methods, semiempirical quantum simulation approaches cover an important system size range where classical potentials are not accu-

rate enough and ab initio computations are not feasible. The tight-binding molecular dynamics (TBMD)⁴ approach thus provides an important bridge between the accurate ab initio quantum MD and classical MD methods.

In computational nanotechnology research, we can use these three simulation methods in a complementary manner to improve computational accuracy and efficiency. Based on experimental observations or theoretical dynamic and structure simulations, we can first investigate a nanosystem's atomic structure. After we finalize the nanoscale system's configurations, we can investigate its electronic behaviors through static ab initio electronic energy minimization schemes⁵ or through studies of the system's quantum conductance⁶ behavior. Investigating the ab initio electronic structure provides highly accurate information about not only the system's thermodynamic minimum energy configurations but also the chemical reactions and charge transfers that occur when two nanoscale systems are brought together or taken apart. Studies of transport behavior are important in designing nanodevices, where the operating characteristics are usually determined by electronic, thermal, acoustic, or chemical signal transfer through the system.

Let's examine some of the main computational techniques. Unfortunately, the range of all possible simulation and computational techniques is too broad to cover comprehensively in this article.

Classical molecular dynamics

Classical MD describes a system's atomic-scale dynamics, where atoms and molecules move while interacting with many of the atoms and molecules in the vicinity. The system's dynamic evolution is governed by Hamilton's classical equation of motion from Newton's second law:

$$d^2\mathbf{R}_i/dt^2 = \mathbf{F}_i = -dV/d\mathbf{R}_i$$

which is derived from the classical Hamiltonian of the system

$$H = \sum \mathbf{P}_i^2/2M_i + V(\{\mathbf{R}_i\}).$$

Each atom moves and acts simply as a particle that is moving in the many-body force field of other similar particles, $\mathbf{F}(\{\mathbf{R}_i\})$, which we can obtain from more accurate quantum simulations. The atomic and molecular interactions describing the dynamics are thus given by classical many-body force-field functions, and we can write the atomic interaction energy function $V(\{\mathbf{R}_i\})$ in terms of pair and many-body interactions that depend on

the relative distances between different atoms.² The atomic forces are analytic derivatives of the interaction energy functions

$$\mathbf{F}_i(\{\mathbf{R}_i\}) = -dV/d\mathbf{R}_i$$

and are used to construct Hamilton's classical equations of motion, which are second-order ordinary differential equations. These equations are approximated as finite-difference equations with discrete time step Δt and are solved by the standard Gear's fifth-order predictor-corrector or Verlet's leapfrog methods. We can perform the simulations under a variety of thermodynamic equilibrium or nonequilibrium conditions, and, depending on the force-field function used, we can describe reactions between atoms and molecules as the molecular building blocks approach each other.⁷

In its global structure, the MD code is applied to a collection of atoms with well-defined potential-energy functions, and the equations of motion are numerically integrated forward in finite time steps by using a predictor-corrector method. We have used the Tersoff-Brenner many-body potential to describe atomic interactions in hydrogen- and carbon-based systems for computational descriptions of carbon nanotubes, and the Tersoff potential for mixed Si/Ge/C-based systems.^{8,9} A major distinguishing feature of the Tersoff-Brenner potential is that short-range bonded interactions are reactive so that chemical bonds can form and break during simulation. The computational cost of the many-body bonded interactions is relatively high compared to the cost of similar methods with nonreactive interactions that have simpler functional forms. So, the overall computational costs of both short-range interactions and long-range nonbonding van der Waals interactions are roughly comparable. An example of the parallel implementation of this classical MD code appears elsewhere.¹⁰

Generalized tight-binding molecular dynamics

The most general approach describes atoms as a collection of quantum mechanical particles, nuclei, and electrons, governed by the Schrödinger equation

$$\mathbf{H}\Phi[\{\mathbf{R}_i, \mathbf{r}_i\}] = E_{\text{tot}}\Phi[\{\mathbf{R}_i, \mathbf{r}_i\}]$$

with the full quantum many-body Hamiltonian operator

$$\mathbf{H} = \sum \mathbf{P}_i^2/2M_i + \sum Z_i Z_j e^2/R_{ij} + \sum \mathbf{p}_i^2/2m_e + \sum e^2/r_{ij} - \sum Z_i e^2/|\mathbf{R}_i - \mathbf{r}_i|$$

where \mathbf{R}_i and \mathbf{r}_i are nuclei and electron coordinates. Using the Born-Oppenheimer approximation, this approach assumes that the electronic degrees of freedom follow adiabatically the corresponding nuclear positions, and the nuclei coordinates become classical variables. This approximation reduces the full quantum many-body problem to the quantum many-electron problem

$$\mathbf{H}[\mathbf{R}_i] \Psi[\mathbf{r}_i] = E_{\text{el}} \Psi[\mathbf{r}_i]$$

where

$$\mathbf{H} = \sum \mathbf{p}_i^2 / 2M_i + \mathbf{H}[\mathbf{R}_i].$$

In the tight-binding method,⁴ an approximation further simplifies the quantum many-electron problem. We assume that the crystal potential is strong such that when an ion captures an electron during its motion through the lattice, the electron remains at that site for a long time before leaking, or tunneling, to the next ion site. During the capture interval, the electron orbits primarily around a single ion uninfluenced by other atoms, so that its state function is essentially that of an atomic orbital. Usually, the electron is tightly bound to its own atom.

The tight-binding wave function is, therefore, constructed by taking a linear combination of localized atomic orbitals, modulated by a Bloch wave-function phase factor for a periodic lattice. This ensures that an electron in a tight-binding level will be found, with equal probability, in any cell of the crystal, because its wave function changes only by the phase factor as one electron moves from one cell to another. The tight-binding method is computationally efficient because we can parameterize the Hamiltonian $\mathbf{H}[\mathbf{R}_i]$. Furthermore, we can easily extract the electronic-structure information from the tight-binding Hamiltonian, which also contains the effects of angular forces in a natural way.

Walter Harrison has attempted to provide a minimal tight-binding theory with only four parameters (in addition to four dimensionless universal constants) that could describe qualitatively a wide range of materials and properties. Although he focused on tetrahedral solids, in later work with Mark van Schilfgaarde, he emphasized the necessity of including the nonorthogonality of the local environment in multicoordinated structures. Those seeking a transferable scheme have generally overlooked this important factor. In our generalized TBMD calculations, we employ a nonorthogonal tight-binding scheme that Menon

and Subbaswami proposed with a minimal number of adjustable parameters, resulting in a transferable scheme applicable to clusters as well as bulk systems containing Si, C, B, N, and H.¹¹

We have applied the generalized TBMD approach to various clusters, surfaces, nanotubes, fullerenes, and bulk carbon- and silicon-based materials. Our generalized TBMD method's advantage is that we can use it to find an energy-minimized structure of a nanoscale system under consideration without symmetry constraints. Sometimes a system's symmetry-unconstrained dynamic energy minimization can help us find the system's global energetic minimum, which is not easily conceptualized on the symmetry consideration alone. The parallelization of the TBMD code involves parallelizing the direct diagonalization (of the electronic Hamiltonian matrix) part as well as the MD part. Parallelizing a sparse symmetric matrix with many eigenvalues and eigenvectors is a complex bottleneck in the simulation of large intermediate-range system and requires new algorithms.

Ab initio simulation methods

The ab initio or first-principles method is a simulation method to solve complex quantum many-body Schrödinger equations with numerical algorithms.⁵ The TBMD method described earlier is another quantum mechanical simulation method based on the linear combination of atomic orbital approximations to describe the quantum mechanical electronic wave functions. Because of the simple basis expansion using atomic orbitals, the TBMD method is approximately 1,000 times more efficient than the ab initio method. However, the ab initio method provides a more accurate description of quantum mechanical behavior of materials properties even though it limits system size to a few hundred atoms. From this viewpoint, MD, TBMD, and ab initio methods form a complementary set of simulation tools to study diverse atomic-scale processes in nanodevice modeling.

Current ab initio simulation methods have a rigorous mathematical foundation provided by two important works.^{12,13} The first proved a theorem that the ground state energy (E_{el}) of a many-electron system is a function of total electron density, $\rho(\mathbf{r})$, rather than the full electron wave function, $\Psi[\mathbf{r}_i]$: $E_{\text{el}}(\Psi[\mathbf{r}_i]) \equiv E_{\text{el}}(\rho(\mathbf{r}))$. The Hamiltonian operator \mathbf{H} and Schrödinger equation are given by

$$\mathbf{H}[\mathbf{R}_i] = \sum \mathbf{p}_i^2 / 2m_e + \sum e^2 / r_{ij} - \sum Z_I e^2 / |\mathbf{R}_I - \mathbf{r}_i| + \sum Z_I Z_J e^2 / R_{IJ}$$

and

$$H[\mathbf{R}_i]\Psi[\mathbf{r}_i] = E_{\text{el}}\Psi[\mathbf{r}_i]$$

where $\{\mathbf{R}_i\}$ and $\{\mathbf{r}_i\}$ are atomic positions and electronic coordinates. The density functional theory (DFT) is derived from the fact that the ground state total electronic energy is a functional of the system's electron density.

Subsequently, Walter Kohn and Lu Sham have shown that the DFT can be reformulated as a single-electron problem with self-consistent effective potential including all the exchange-correlation effects of electronic interactions:

$$H_1 = \mathbf{p}^2/2m_e + V_H(\mathbf{r}) + V_{\text{XC}}[\rho(\mathbf{r})] + V_{\text{ion-el}}(\mathbf{r}),$$

$$H_1 \psi_i(\mathbf{r}) = \varepsilon_i \psi_i(\mathbf{r}), i = 1, \dots, N_{\text{tot}}$$

$$\rho(\mathbf{r}) = \sum |\psi_i(\mathbf{r})|^2.$$

This single-electron Schrödinger equation is called the Kohn-Sham equation—the local density approximation (LDA) approximates the unknown effective exchange-correlation potential. This combined method has successfully predicted materials properties without using any experimental inputs other than the identity of the constituent atoms.

For practical applications, the combined DFT-LDA method has been implemented with a pseudopotential approximation and a plane wave basis expansion of single-electron wave functions.⁵ These systematic approximations reduce the electronic structure problem to a self-consistent matrix diagonalization problem. Over the last three decades, the simulation method has rapidly improved from the iterative diagonalization method to the Car-Parrinello MD method³ to the conjugate gradient minimization method. Car-Parrinello MD has significantly improved the computational efficiency by reducing the iterative diagonalization method's N^3 scaling down to N^2 scaling. The conjugate gradient minimization method has further improved this efficiency by an additional factor of two to three.⁵ A popular DFT simulation program is the Vienna Ab Initio Simulation Package, which is available through a license agreement.¹⁴ Other useful DFT simulation programs include one for C++ and a commercial package from Molecular Simulation. With these and other widely used DFT simulation packages, the ab initio simulation method is a major computational materials research tool.

Quantum conductance in nanoscale systems

We can calculate quantum conductance as a generalization of the transmission amplitude $T(E)$ of an incident electron with energy E in a simple 1D potential barrier problem. The Landauer expression is generally used to obtain quantum conductance from the $T(E)$ —which is obtained with the Green's function formalism⁶—as a function of the injected electron energy.⁶ A realistic treatment of a nanotube interaction with metal electrodes must involve a judicious construction of the Green's function and is an involved process. To maintain consistency in the simulations, it is proper to use the tight-binding formulation for both the Hamiltonian and the Green's function. The tight-binding Hamiltonian described earlier consists of $N \times N$ matrices, where $N = N(\text{at}) \times N(\text{orb})$; $N(\text{at})$ is the number of atoms in the embedding subspace and $N(\text{orb})$ is the number of orbitals on each atom. Contrary to previous theoretical works on quantum transport that use $N(\text{orb}) = 1$ (only one pi-electron orbital per atom) for accuracy, we use $N(\text{orb}) = 9$. This includes 1s, 3p, and 5d orbitals for the Ni (a representative material for metal leads) interface and $N(\text{orb}) = 4$ for C atoms. Other researchers have used this Hamiltonian to treat transition metal systems and their interactions with carbon fullerenes and nanotubes.¹⁵

We have used the same tight-binding Hamiltonian to perform full symmetry-unconstrained MD relaxations for SWNT systems. Consideration of the atomic relaxation is essential and has given results significantly different from cases where dynamic relaxation was not allowed. In addition, quantum conductance simulations are generally complemented by ab initio calculations of the electronic density of states or the energy differences between the highest occupied molecular orbital and lowest unoccupied molecular orbital states. Features observed in the conductance are generally explained by the qualitative movements of the density of states or highest occupied molecular orbital (lowest unoccupied molecular orbital) states with respect to the system's fermi level.

For quantum conductivity calculations, the Green's function formalism embeds a nanotube between host lattices consisting of transition metal atoms forming the semi-infinite leads at the two ends. A boundary surface S separates the embedded system (tube) from the host lattice (leads) with the Green's function of the host satisfying the Dirichlet's boundary condition on S .¹⁵ The lead-tube interaction is incorporated through the introduction of an electron self-energy term in

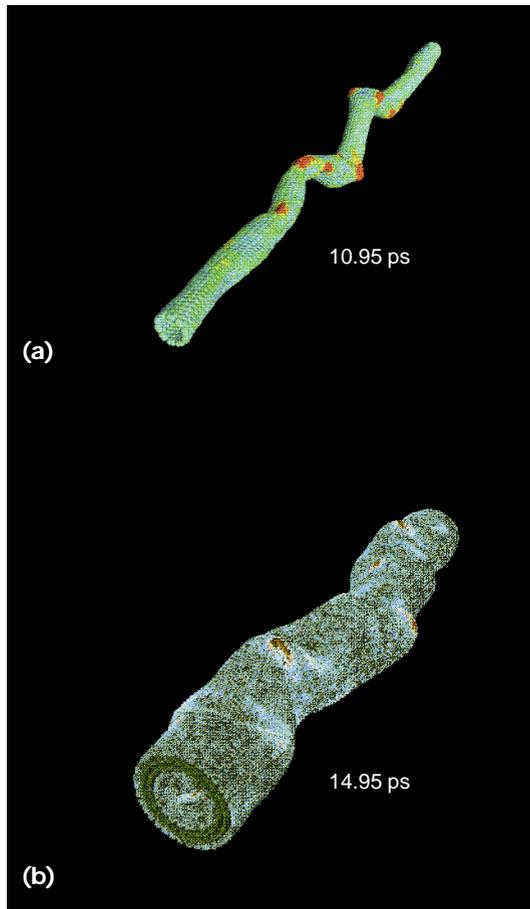


Figure 2. Axial compression and plastic collapse of (a) a single-walled carbon nanotube and (b) a multiwalled carbon nanotube.

the formalism. Each metal-lead has a self-energy term. Although self-consistent calculations are desirable, the system's size (the number of atoms as

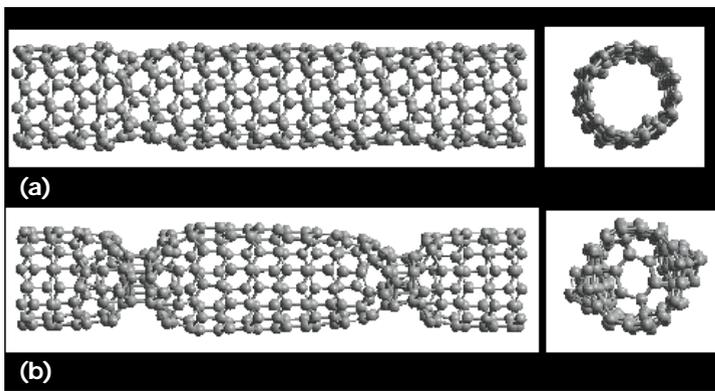


Figure 3. A 12 percent axially compressed (8, 0) nanotube at the (a) beginning and (b) end of a spontaneous local plastic collapse, which is driven by diamond-like bonding transitions at the collapse's location (the cross-section in (b)).

well as the use of many orbitals for each atom) makes this prohibitively expensive. Previous self-consistent calculations of quantum conductance have involved only very small systems (typically fewer than 15 atoms).¹⁶ The current method's unique features are that the Hamiltonian used in calculating the conductivity is identical to the one used in performing TBMD simulations for relaxing all structures considered.

Applications in a nanoworld

Computational nanotechnology has played an important role in explaining some recent experimental observations and predicting structures (or properties) that were later fabricated (or measured) in experiments. Let's examine some applications.

Nanomechanics of C and BN nanotubes

Since their discovery in 1991,¹ SWNTs and MWNTs have displayed exceptionally strong and stiff mechanical characteristics along the nanotube's axis and flexible characteristics along the normal to the tube's axis.^{10, 17-19} Researchers have tried to exploit nanotubes' strengths as reinforcing fibers in nanotube-polymer composite materials.²⁰

Initial investigations, using classical MD simulations with the Tersoff-Brenner potential, showed that the tubes were extremely stiff under axial compression and that the system remained within the elastic limit even for very large deformations (up to 15 percent strain).^{10,17}

Nonlinear elastic instabilities (with the appearance of fin-like structures) occur during these deformations, but the system remains within the elastic limit and returns to the original unstrained state as soon as external constraining forces disappear. As Figure 2 shows, when compressed beyond elastic limits, the SWNTs and MWNTs undergo sideways buckling, and plastic deformations occur mainly through extreme bending situations in the sideways-buckled tubes. The red regions in the sideways-buckled tubes are the regions under extreme stress. The garden-hose-type sideways buckling of thick MWNTs also occur in microscopic images of nanotubes embedded in polymer composite materials.²⁰ Deformations such as plastic collapses or fractures of thin nanotubes without any buckling also appear in experiments,²⁰ but these deformations have never appeared in classical MD simulations with the Tersoff-Brenner potential.^{10,17}

To explain this discrepancy, we repeated the

simulations with a more accurate quantum generalized TBMD description of nanotube nanomechanics.¹⁸ For an (8, 0) carbon nanotube, within low values of compressive strain (less than 8 percent strain), the classical MD results reasonably agree with the quantum simulation results. Significant differences, however, start to occur for compressive strain larger than 8 percent. At a 12 percent strain (see Figure 3a), the structural deformation occurs asymmetrically near the two rigidly held ends with small changes in an otherwise circular cross-section of the tube. Strain relaxation in the center (highly strained) region of the tube drives the atoms at the locations of the deformations to gradually collapse inward (see Figure 3b). Fourfold coordinated diamond-like bonds form, and the newly formed sp³ (diamond-like)-type bonds further pull the structure inward.

We have also carried out similar simulations and analysis of axial compression of boron-nitride (BN) nanotubes. This study involves more variations in the physics and chemistry of the system involved and has led us to predict a novel anisotropic compressibility of BN nanotubes. The main differences are due to two prominent structural differences between C and BN nanotubes:²¹

- *Bond frustration effect:* The presence of B-B and N-N bonds in BN nanotubes makes them structurally unstable, because they are energetically unfavorable.
- *Bond rotation effect:* Structural relaxation causes each BN bond to be slightly rotated such that each N is rotated out and B is rotated in to a BN nanotube's surface (see Figure 4).

On the basis of the bond frustration effect, we have predicted that the zigzag BN nanotubes are more stable and can be easily made in experiments.²¹ Recent experiments confirm our prediction, and the zigzag arrangement dominates BN nanotubes in experiments.²²

The main effect of rotated BN bonds on nanomechanics is to give an anisotropic mechanochemical characteristic to zigzag BN nanotubes. Because the BN bonds are parallel to the tube axis in zigzag nanotubes, the strained BN bonds show a novel anisotropic plastic collapse under axial compression. In Figure 5a, the surface of a BN nanotube with 14.5 percent compression shows a localized sawtooth or rippled structure in which the B atoms have further rotated inward and the N atoms have further moved outward.²³ The structure's spontaneous

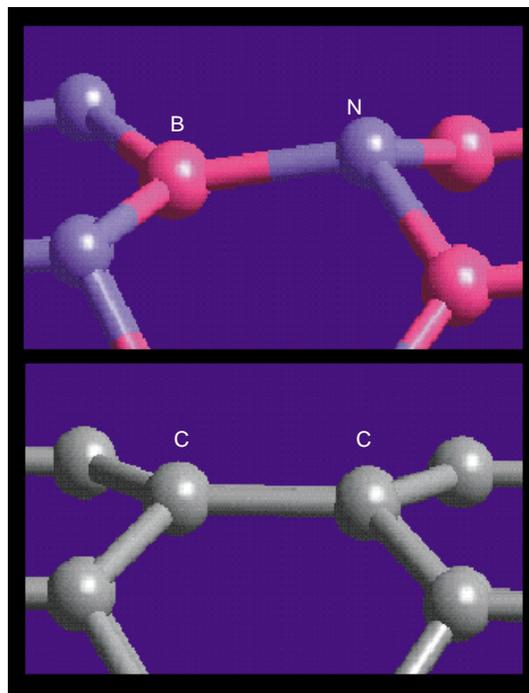


Figure 4. (a) A rotated boron-nitride bond and (b) a nonrotated carbon-carbon bond.

relaxation leads to a plastic deformation or collapse, but with an anisotropy only toward the right end of the compressed tube (see Figure 5b). This anisotropy is driven by a strain release that occurs preferentially toward N atoms as the leading side of rotated BN bonds.²³ A correlated sliding of N atoms farther outward and B atoms farther inward facilitates this anisotropic process.

Based on the anisotropic strain release and the resulting plastic deformation mechanism, we can propose a hypothetical composite material reinforced by parallelly aligned zigzag BN nanotubes. The material exhibits a nanostructured “skin” effect in that the material has an anisotropic response to external axial strains. When subjected to large external axial strains, the material reacts by minimizing the damage to the inner-core side, while transferring all the damage to the outer skin or surface side. This skin effect could play an important role under external shock-impulse-induced damage because the composite material will not have enough time to develop a long-wavelength geometric instability to absorb the effect of normal uniaxial shock impulses. Such a hypothetical material, if synthesized, could have useful applications in the transportation, aerospace, defense, and armor industries.

This set of simulations for nanotube mechanics also shows that in the nanoworld, simulations not

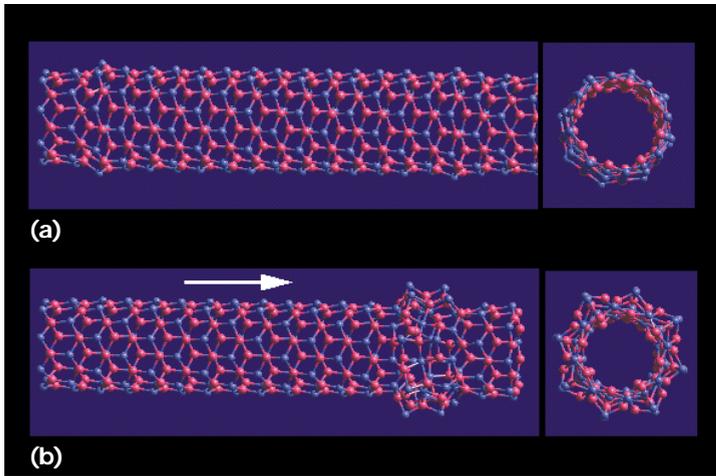


Figure 5. An (8, 0) boron-nitride nanotube axially compressed by 14.5 percent strain (a) before and (b) after the anisotropic plastic collapse.

only can verify and explain experimental observations—they also can predict new phenomena. We don't expect to observe the phenomena predicted by the quantum TBMD—such as anisotropic collapse in a BN nanotube²³—in any continuum mechanics or classical MD-based descriptions because of the explicit physical and chemical nature of the atomic interactions involved. Future experimentalists might try to exploit newly predicted phenomenon such as the nanostructured skin effect to develop lightweight, high-strength, functionally smart materials.

Molecular electronics

The possibility of using carbon in place of silicon in electronics has generated considerable enthusiasm as well. Could we use individual (or bundles of) nanotubes as quantum molecular wires for interconnects in future electronic and computing devices? Many independent studies support ballistic electron transport through individual nanotubes; researchers consider this one of the reasons why nanotubes exhibit high current density as compared to other materials at a similar scale. Additionally, researchers have also explored nanotubes for nanoscale field-effect transistors and nanoelectromechanical switching devices.²⁴

Several authors have recently investigated the possibility of connecting nanotubes of different diameters and chiralities in nanotube heterojunctions²⁵ as examples of carbon nanotube-based molecular electronic devices or switching components. The simplest way to connect two dissimilar nanotubes is by introducing pairs of heptagons and pentagons in an otherwise per-

fect hexagonal graphene lattice structure. The resulting junction still contains threefold coordination for all carbon atoms; the heterojunction between a semiconducting and a metallic nanotube could act as a rectifying diode. Such two-terminal heterojunctions or rectifying diodes were first postulated theoretically²⁵ and have recently occurred in experiments.²⁶ Two-terminal nanotube junctions, however, are difficult to create in experiments, much less to use in any molecular electronic circuitry for switching.

There are two ways to create more-than-two-terminal nanotube heterojunctions. First, connect different nanotubes through molecularly perfect but topological defect-mediated junctions.²⁷ Second, lay crossed nanotubes over each other and form the physically contacted or touching junctions.²⁸ The difference in the two approaches is the nature and characteristics of the junctions that form the device. In the first case, nanotubes are chemically connected through bonding networks, forming a stable junction that could possibly give rise to a variety of switching, logic, and transistor applications in the category of monomolecular electronic or computing devices.²⁹ In the second case, the junction is merely through a physical contact and is amenable to changes in the contact's nature. The main applications in the second category will be in electro-mechanical switches and sensors.²⁸

We were the first to propose the structures of a variety of carbon nanotube T- and Y-junctions as models of three-terminal nanoscale monomolecular electronic devices.^{27,30} Think of our initially proposed T-junctions as a specific case of a family of Y-junctions in which the two connecting nanotubes are perpendicular to each other. We proposed and studied a variety of T-junctions for electronic characterization (see Figure 6a). The Y-junctions pose a different kind of challenge for three-point junction formations: the pentagon–heptagon defect pair rule does not apply to their formation. Instead, the formation of large angle bends is explored through octagon–pentagon defect pairs, which gives greater flexibility in the Y-junction formation. The number of octagonal defects equals the number of pentagonal defects in the junction region, and symmetric obtuse angle Y-junctions are formed this way (see Figure 6b).

Progress in the recent experimental feasibility of the hardwired or chemically connected junctions has given a new thrust to this slowly expanding field of carbon nanotube-based monomolecular electronic devices. Earlier occasional

experimental observations of carbon nanotube Y-junctions did not attract much attention for electronics applications. This was mainly due to the difficulties associated with their synthesis and the complexities of their structures. For the Y-junctions to be useful from the nanoscale electronic device perspective, controlled and high-yield production of these junctions is required. Recently, experimenters have succeeded in developing template-based chemical vapor deposition³¹ and pyrolysis of organometallic precursors with nickelocene and thiophene³²—techniques that allow the reproducible and high-yield fabrication of MWNT Y-junctions.

We have computed quantum conductivity on a variety of carbon nanotube Y-junctions that also show current rectification because of changes in the bias voltage. Although all the Y-junctions considered in our work show current rectification, the degree depends on the types and natures of Y-junctions considered—some show good rectification whereas others show small leakage currents. The presence of rectification indicates, for the first time, the formation of a nanoscale molecular rectifying switch with a robust behavior that is reproducible in a high-yield fabrication method. The molecular switches thus produced can easily function as three-terminal bi-stable switches that a control or “gate” voltage applied at a branch terminal can control. If the gate or control terminal can be insulated from the current flowing across the junction in the other two terminals, the three-terminal nanotube junctions such as the Y-junctions could be used in standard nanoscale monomolecular transistor or amplifier applications as well. The physical nature and the response characteristics of such devices, however, is complex and might differ from standard devices.

The transport behavior of all Y-junctions that we have simulated shows current rectification. However, the possible role of the topological defects at the junction in robustly insulating the current flow in the primary channel is not entirely clear. Charge calculations for the topological defects suggest that the heptagonal rings have a positive charge. We can expect the positions of the defects relative to the junction, therefore, to factor in rectification. The small current leakage might be due to the different location of heptagonal defects for different Y-junctions. Another possible factor could be the constructive or destructive interference of the electronic wave functions through two different channels at the junction’s location. We further investigated this by exploring the struc-

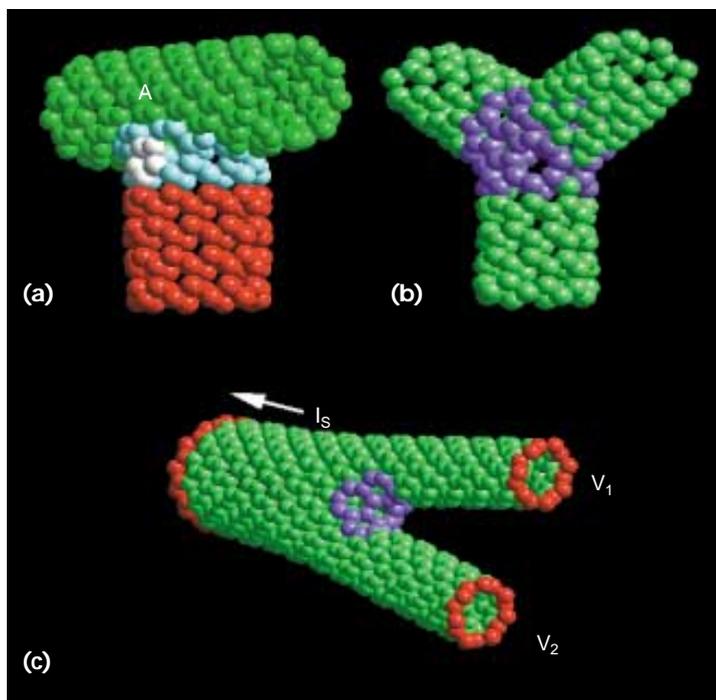


Figure 6. (a) A carbon nanotube T-junction connecting a zigzag nanotube (red) to an armchair (green) nanotube through defect rings (blue and white); (b) an obtuse-angle symmetric Y-junction nanotube connecting (8, 0) nanotubes in all three branches; and (c) an acute-angle Y-junction connecting a (14, 0) nanotube to two branches of (7, 0) nanotubes.

ture-induced asymmetry across the two branches in a junction and found the nature of switching to be ballistic.^{31–34}

In considering the architecture for molecular-electronic-based devices and computing systems, we need not constrain ourselves to the specifications of silicon-based devices, circuitry, and architecture. For example, we could consider an architecture of a 3D network of chemically interconnected nanotubes where nodes at the junction serve as devices and switches and are self-connected to each other through nanotubes. It is not easy to conceptualize the possible fabrication pathways for such networks or the new computing or logic paradigms suitable for such network-based extended architectures. A possible alternative architecture could be based on the structure and functioning of dendritic neurons in biological neural logic and computing systems.

Figure 7 shows an example of a carbon nanotube Y-junction-based biomimetic dendritic neural tree. The tree in the figure has four levels of branching structure and is made of 14 carbon nanotube Y-junctions. Such a structure is conceptually amenable to fabrication through the template-

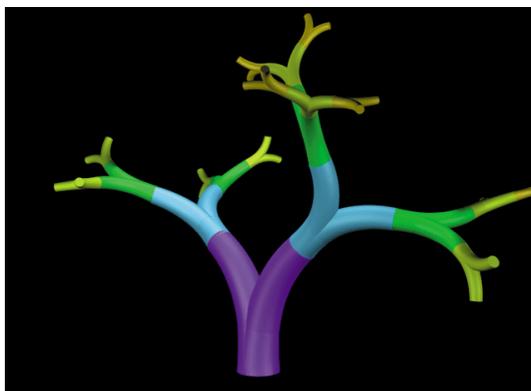


Figure 7. A four-level dendritic neural tree made of 14 symmetric Y-junctions.

based chemical vapor deposition method and provides a first model of biomimetic neural networks made of SWNTs and MWNTs.³⁵ The branching and switching of the signals at each nanotube Y-junction could be similar to what happens in a biological neural network, and once fabricated, such a “tree” could be trained to perform complex computing and switching applications in a single pass. Also, the signals propagated, branched, and switched on such a network need not be restricted to the “electronic” regime. Similar logic and switching functions might also be possible with thermal, acoustic, and chemical signals as well. Our work is progressing on testing some of these far-fetched ideas with computational nanotechnology-based simulations.

Endofullerenes as qubits for solid-state quantum computer design

Modern computer design is based on sequential processing of numerical bits (zeros and ones), which form the basis of the well-known von Neumann architecture. Quantum computation is based on a fundamentally different concept of quantum bits (qubits), which are quantum states of a two-level system such as an electron or nuclear spin of an atom. A quantum computer with more than 20 to 30 qubits can outperform conventional classical computers for a certain class of computing tasks, dramatically increasing computing power.³⁶ Recent experimental demonstrations of nuclear magnetic resonance (NMR) quantum computation has already proven the feasibility of a device implementation in a real quantum computer.³⁷ However, these experiments are limited in scaling and would not be suitable as a platform to develop highly scalable quantum computers.

To overcome the scalability problem of NMR quantum computers, Bruce Kane has proposed a solid-state quantum computer based on ³¹P dopant atoms in bulk crystalline silicon.³⁸ The nuclear spin of a phosphorous atom with atomic weight 31 (³¹P) is used as a solid-state qubit, and the qubit state is controlled by hyperfine coupling to the weakly bound donor electron of the ³¹P atom in a silicon lattice. The quantum computer can therefore be continuously scaled using the electronic device industry’s microfabrication technology. However, there is a challenge in realizing Kane’s conceptual quantum computer design. Experimentally, we do not know how to place a single dopant atom at a precise position in a silicon lattice or how to prevent a dopant atom’s diffusion. Current microfabrication technology applies a δ -doping technique to control the depth of dopant atoms; the positioning of the atoms cannot be controlled to atomic precision. Furthermore, significant dopant atom diffusion occurs even at very low temperatures owing to the transient enhanced diffusion mechanisms (induced by silicon vacancies and self-interstitial defects).

Recently, we proposed a possible solution to these positioning and diffusion problems using carbon-based nanotechnology.³⁹ In this new design, a carbon diamond lattice replaces the silicon diamond lattice as a host material for ³¹P dopant atoms. This change of host material solves both positioning and stability problems. The basic idea is to fabricate a diamond nanocrystallite with a ³¹P dopant atom at the center using multishell fullerene. The sequence of fabrication steps for nanocrystallite is as follows. First, encapsulate a ³¹P atom within a C₆₀ fullerene through ion implantation methods to create an endofullerene, P@C₆₀, as demonstrated in a recent experiment.⁴⁰ Second, use the P@C₆₀ as seed material to grow a “bucky onion,” a concentric multishell fullerenes, encapsulating the endofullerene. Third, use an e-beam or ion irradiation on the bucky onion to convert the inner-core graphitic layers into a compressed diamond nanocrystallite. An experiment has shown that this third step produces a compressed diamond nanocrystallite with a 2- to 10-nm diameter.⁴¹

The position control of a ³¹P atom qubit is feasible by fabricating arrays of 2- to 10-nm nanocrystallite (with ³¹P at the center) qubits in any host dielectric material including diamond lattices. The dopant atom’s stability is ensured by much higher formation energies of vacancy (7 eV) and self-interstitial (~10 eV) defects in dia-

mond than those in silicon lattices. The P atom's stability is further enhanced by its stability at substitutional sites relative to interstitial sites (by 15 eV). Because of higher formation energies, vacancy and self-interstitial defects are not likely to form during the graphite-to-diamond transformation process at the inner core of bucky onions to suppress the transient enhanced diffusion mechanism of P atoms. Figure 8 shows the results of ab initio simulations of P@C₆₀ and a ³¹P doped at the center of a diamond nanocrystallite. The figure shows the planar valence electron density and the ³¹P donor electron density in the (111) plane in a diamond lattice in the two cases.³⁹

Nanotube-based sensors and actuators

As we mentioned earlier, carbon nanotubes have different electronic properties depending on their chirality vector, ranging from metals to semiconductors (1 eV bandgap). Recent theoretical and experimental works have proven that SWNTs are extremely sensitive to gas molecules.⁴² In the experiments, a semiconducting nanotube's conductivity changes as the nanotube is exposed to a miniscule amount of certain gas molecules. In the ab initio simulations, gas molecules induce a charge transfer, which causes doping effects on semiconducting nanotubes.^{43,44} The gas molecules are adsorbed into the nanotube's surface, and each molecule induces small amounts (about 0.1 e) of electron transfer so that the nanotube becomes a *p*-type doped semiconductor.

Experiments have shown that the nanotube sensor can detect ppm-level gas molecules at room temperature, which opens the possibility of developing a nanotube biosensor operating at physiological temperatures. An ab initio study of water adsorbed on an SWNT shows a purely repulsive interaction without any charge transfer—an SWNT can be fully immersed in water and maintain its intrinsic electronic properties.⁴³ A recently developed experimental technique that attaches a protein on a nanotube's surface through noncovalent bonds shows a very promising direction toward developing nanotubes for biosensor applications.

Carbon nanotubes also show a strong electro-mechanical coupling in our recent simulations.⁴⁵ As

the cross-section of an (8,0) SWNT is flattened up to 40 percent, the nanotube's bandgap decreases from 0.57 eV and disappears at 25 percent deformation. As the deformation further increases to 40 percent, the bandgap reopens and reaches 0.45 eV. We can apply this strong dependence of SWNT band structure on the mechanical deformation to develop nanoscale mechanical sensors. Furthermore, mechanical deformation can control the electronic excitation by static electric fields or electromagnetic waves. A recent ab initio study of polarons in SWNTs shows that the electron-hole pair creation can induce a tube length change, leading to an optical actuation mechanism of nanotube mechanical properties. The strong coupling of electronic, optical, and mechanical properties of SWNT offers a great opportunity to develop novel nanodevices.

Much of the recent progress in computational nanotechnology is in the experimental biomolecular motors arena. Researchers have gained significant understanding about how the natural biological motor systems work and how to create interfaces of nanoscale biomolecular motors with synthetic materials in solution-phase environments.⁴⁶ Means to power these machines through biomimetic physical and chemical phenomenon are also under investigation. Ultimately, we might see nanoscale synthetic machines and motors that are powered and controlled through external laser, electric, or magnetic fields and that could operate in chemical solution phases or inert gas environments.^{47,48}

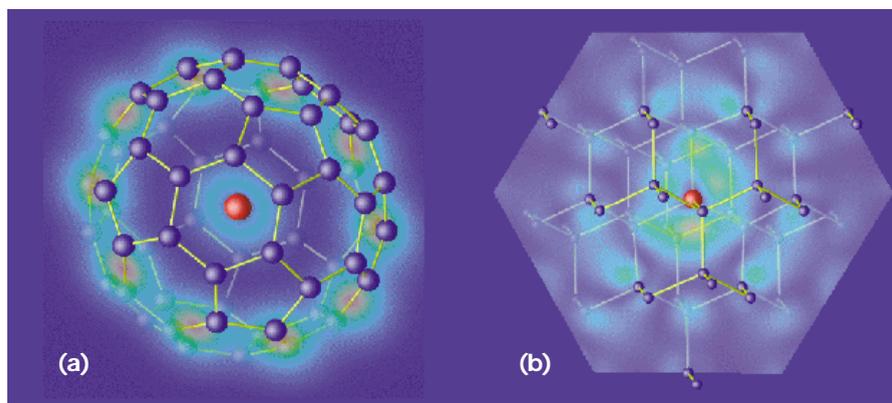


Figure 8. The P atom's (a) stable position and valance electron charge density in a C₆₀ fullerene and (b) its position and weakly bound donor electron density after it has been encapsulated in a diamond nanocrystallite.

A final issue concerns building the world atom-by-atom from the bottom up—the holy grail of molecular technology. Experimentally, certain areas could contribute significantly toward advances in this direction. These areas are nanomanipulation and control of atomic- and molecular-level entities on solid, 3D surfaces and self-assembly of molecular-scale materials where chemical and topological structural forces can guide chunks of nanoscale materials toward larger functional materials structures. Computational nanotechnology can and does contribute significantly to this by simulating the assembly of building-block materials. **SE**

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