Chapter 2

INVESTIGATIVE TOOLS: THEORY, MODELING, AND SIMULATION

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2.1   VISION

A critical issue for nanotechnology is that the components, structures, and systems are in a size regime about whose fundamental behavior we have little understanding. The particles are too small for direct measurements, too large to be described by current rigorous first principle theoretical and computational methods, exhibit too many fluctuations to be treated monolithically in time and space, and are too few to be described by a statistical ensemble. Fundamental understanding and highly accurate predictive methods are critical to successful manufacturing of nanostructured materials, devices, and systems.

2.2   CURRENT SCIENTIFIC AND TECHNOLOGICAL ADVANCEMENTS

In the field of theory, modeling, and simulation (TM&S), the most significant advancements applicable to nanotechnology have been associated with the introduction of more powerful computers and corresponding advances in software and algorithms, and to a lesser degree, with the broaching of new theories. These have enabled the merging of several different types of computational techniques (for example, quantum chemical and molecular dynamics) to provide high-fidelity simulations of nanoscale objects based on first principles theory.

2.3   GOALS FOR THE NEXT 5-10 YEARS: BARRIERS AND SOLUTIONS

Even though it is difficult today to fully model nanoscale systems, it is clear that TM&S is the key enabling field for the following:

- Reducing the time needed to design new materials

- Developing nanoscale devices from the new materials

- Increasing the reliability and predictability of the operation of the new devices

- Designing and optimizing new nanoscale technologies

As is well known from conventional silicon technology, TM&S immediately leads to financial savings in terms of time expended, capital invested, and the quality of the final product. TM&S is an enabling field in that it can provide new levels of understanding and provide numerical values when experimental results are not available. Furthermore, modeling and simulation are often needed to properly interpret an experimental

measurement, due to the complexity of the measurement or the averaging done under the experimental conditions. In addition, TM&S is essential to continuing to exploit the living cell's nanosystems as models for future developments in nanotechnology. Recall that much of our current inspiration for the design of many nanodevices and systems has been based on our understanding of nature's nanomachines, proteins.

However, TM&S as applied to nanosystems needs significant advances in order to be successful. For example, quantum chemical and molecular theory and simulation will be required to offer fundamental insights and provide predictability methods for nanoscale material properties such as thermophysical, thermochemical, electrical, magnetic, and rheological behavior. Optimization of nanoscale materials or devices will require exploration of thousands of design alternatives prior to synthesis. Properties of nanoscale devices embedded in larger-scale environments need to be modeled; hence models must traverse the various scales (molecular, nano, meso, and macro) that constitute a working device and its manufacture.

Significant technical issues in modeling nanomaterials and nanodevices add to the complexity of the models. One cannot just consider the individual components; nanoscale devices need to be understood in the context of their environment and as elements of architectures that can include meso-scale and macro-scale entities. An example of such a hierarchy for electronics is

<div align="center">

Materials → Devices → Circuits → Systems → Architectures

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The tools that are the mainstay of the CMOS-based microelectronics industry today, such as SPICE, PISCES, and SUPREM, have no applicability in the coming nanoelectronic era. We need to develop new tools that connect across all of the various scales in order to enable the electronics industry to advance into the nano era. An example of new technology is that the ever-increasing speed of computers has enabled us to find numerical solutions to several differential equations, including Shockley's semiconductor device equations, Maxwell's equations, Boltzmann's equation, and Schroedinger's equation (for given potentials), all with realistic boundary conditions in three dimensions.

Enhanced computing capability thus enables the researcher to simulate electronic devices beyond the conventional way in which the device function has been partitioned into various subfunctions and sections. The physics of these sections was once explored using modest numerical tools such as integration and compared to experiments; the connection to other device sections and creative optimization was entirely left to the researcher. It is now possible to treat the device as a whole, and the interactions between the various device functions, parts, and sections can be optimized numerically, resulting in important improvements that are really needed from an engineering point of view.

For future nanostructure simulation, these new tools and methods must be combined and linked to an atomistic understanding. An interdisciplinary effort will be required to combine solutions of the equations of Shockley and Boltzmann (as done now in electrical engineering) with atomistic density functional theory (as done now in chemistry and physics). Unique opportunities exist here for the merging and novel use of existing knowledge.

There are many length and time scales that are important in nanotechnology. The length scale goes from 10 Å to 10^4 Å, which encompasses 10^2 to 10^{11} particles, yet one must still be faithful to the atomic scale, since nanomaterials will often be made up of small molecules. Because the particles are small, surface effects are crucial. Interactions with other species are also crucial, as are interactions with the environment; this means that researchers must consider using the chemical potential where appropriate. There are also many different types of time scales, ranging from 10^{-15} s to several seconds, so consideration must be given to the fact that the particles are actually undergoing fluctuations in time and to the fact that there are uneven size distributions. To provide reliable results, researchers must also consider the relative accuracy appropriate for the space and time scales that are required; however, the cost of accuracy can be high. The temporal scale goes linearly in the number of particles N, the spatial scale goes as $O(NlogN)$, yet the accuracy scale can go as high as N^7 to N! with a significant prefactor. A critical problem is that there are fundamental limitations on the ability of parallel supercomputers to solve the time problem, because this is dependent on the speed of the processor as well as on the speed of the switch. Furthermore, much of the action on the nanoscale takes place at the transition/interface between quantum mechanics and classical mechanics, a region for which not many methods have been developed and which has not been explored in detail.

2.4 SCIENTIFIC AND TECHNOLOGICAL INFRASTRUCTURE

The TM&S areas that must be developed in order to make needed advances in nanoscience include mesoscale theories; complexity theory; multiscale methods, including advances in applied mathematics; and order-N methods for computational efficiency—all with the required accuracy. In addition, there is a critical need for development of accurate, transferable force fields for molecular simulations for all atoms in the periodic table. The complexity of molecular systems also demands new methods for optimizing complex structures that will have application in predicting the self-assembly of nanostructured materials; an example of this is *de novo* protein folding. Furthermore, all of these methods need to be interoperable, and the data from one calculation must be able to be readily used by another, in the correct form, with the correct accuracy and uncertainties included. For example, the computational chemistry/ electronics/micromechanics/physics (CCEMP) approach needs to be developed beyond its current capabilities, since self-consistent combinations of the relevant differential equation systems need to be solved. As another example, a laser diode demands the solution of the Shockley equations, the Maxwell equations, and the Schroedinger equation for the quantum well, all fully and self-consistently coupled.

Even if such solutions were possible with current computers—and in three dimensions they are not—this still would not solve all nanostructure problems. The various methods must be integrated and made to be easily used by a broad range of scientists and engineers in order to have an impact on device design. Achieving this will necessitate development of modern collaborative problem solving environments (CPSE), as well as shared databases. A CPSE is really needed in order to have a geographically dispersed group of people all working on the same problems and developing a common set of theories and software. We must build smart software that automatically adjusts the level of calculation for the best balance of speed and accuracy; we must build interfaces so that

an engineer can design systems on a computer without a detailed understanding of every aspect of quantum mechanics, force fields, molecular dynamics, mesoscale, finite element analysis, etc.; the designers also need answers fast enough to make decisions. An example of a CPSE would be an Internet platform that makes the existing simulation tools (e.g., band-structure calculations, Poisson solvers, etc.) available to everyone. This should include (at least a list of) solvers of Maxwell's, Shockley's (devices), Boltzmann, and Schroedinger equations.

Clearly, most areas of nanotechnology will be dramatically improved by increased emphasis on simulation. However, there can be some misunderstanding of the nature of the critical needs in this area. In general, there is a strong emphasis on computer science, particularly the acquisition of massively parallel hardware and software compatible with massive parallelism. Such supercomputer facilities are essential for the large-scale simulations required to advance the technology and for providing a number of the solutions required.

It is also important to support development of theoretical methods, which are just as important in this area as is developing the software. We must also train students in TM&S for nanotechnology in a wide range of areas, including chemistry, physics, materials science, applied physics, biology, computer science, chemical engineering, and electrical engineering, and provide them with backgrounds in ceramics, polymers, semiconductors, metal alloys, catalysts, and other areas.

2.5 R&D INVESTMENT AND IMPLEMENTATION STRATEGIES

A concerted coordinated interagency basic research effort in nanoscience and technology would have enormous synergy with the presidential interagency initiative Information Technology for the Twenty-First Century (IT^2). Nanoelectronic devices are the *only* apparent route to creating the computing and networking breakthroughs needed to fulfill the ultimate goals of the IT^2 initiative. Likewise, the extraordinary advances envisioned in the IT^2 initiative provide the computer power and software environments that permit computational modeling and simulation on the extreme scale needed to understand, design, and optimize new nanoscale devices. Thus, realization of the goals of the IT^2 initiative is crucially dependent on success in an aggressive national initiative in nanoscale science and technology; likewise, the full potential of a national initiative in nanoscale science and technology cannot be achieved without the development of new computational and simulation capabilities made possible through the high-performance computing and networking resources provided by the IT^2 initiative.

2.6 PRIORITIES AND CONCLUSIONS

Priorities

- Develop simulations that embody multiscale and coupled multiphenomena descriptions. Special attention should be given to larger systems of atoms and molecules and to simultaneous simulation of more than one aspect (mechanical, electronic, etc.).

- Advance outstanding theories, such as nucleation, charging, electron transport, mechanical cracking, chemical reactions in special environments, and multibody processes in order to significantly improve simulations.

- Take advantage of outstanding opportunities for development of theories and simulation methods by studying nanostructures. This may provide ground for new theories that can be used in other fields.

- Maintain continuous assessment and interaction among researchers doing simulations on various aspects of nanoscience and engineering.

- Encourage cross-disciplinary research (e.g., nanoelectronics, thermodynamics, ehcmistry, mechanics, biological processes, and others) and education in order to enable future developments in nanotechnology.

2.7 EXAMPLES OF CURRENT ACHIEVEMENTS AND PARADIGM SHIFTS

2.7.1 Scales and Scaling of Computational Complexity for Molecular Calculations on Nanoparticles

Contact person: D. Dixon, Pacific Northwest Lab.

One of the important issues in computational science is the scaling of the computation. As shown in Figure 2.1(a), scaling must be considered in three different dimensions. Figure 2.1(b) and (c) show details of the different experimental and computational methods that can be used to study the temporal axis (b) and the spatial axis (c) (Alivisatos et al. 1998).

In (a), the X axis represents spatial scaling and ranges from the size of an atom (~1 Å) to the size of a nanoparticle (~1 μm). The computational scaling for chemical calculations along this axis is reflected by the need to treat Coulomb interactions, and this scales between n and n^2, with the best being O(NlogN) where N is the number of particles. With present treatments of dynamics, temporal scaling is given along the Y axis and is linear in the number of particles; however, there is a significant dynamic range because atomic motions are on the order of 1 fsec which means that 15 orders of magnitude are needed in order to reach a time of 1 sec, still fast for many macroscopic processes. The Z axis represents the accuracy of the calculation. There is an increased need for accuracy in the computation as one strives for tighter design principles, providing new insight, and minimizing the number of expensive experiments. It is now possible to go beyond the old limit of "chemical accuracy" of 1 kcal/mol. The scaling on the Z axis is much worse in terms of the scaling with the number of particles. Actually, the scaling is in terms of the number of basis functions, with between 50 and 100 basis functions needed for each particle. The scaling goes as N^m, with m=7 for very high accuracy calculations, and can go to N! for full configuration interaction calculations. Even accuracies of 5 to 10 kcal/mol may require calculations scaling with m=5. The drive for larger computer resources is driven by the need to go to larger sizes, longer times, and higher accuracy.

Although there are classes of problems in nanoparticles that are accessible via established computational and experimental approaches, it is important to emphasize that the questions that become relevant are often not obtainable in terms of well-developed approaches. Figure 2.1 (b) and (c) show why this is so, illustrating the appropriate time

and length scales for the understanding of structure and properties of nanoparticles. There are many choices of experimental methods for the preparation and characterization of particles dependent on the length and time scale, and the same is true for theoretical/computational studies. Figure 2.1 (b) characterizes the different temporal regimes that can be studied by using dynamics theory.
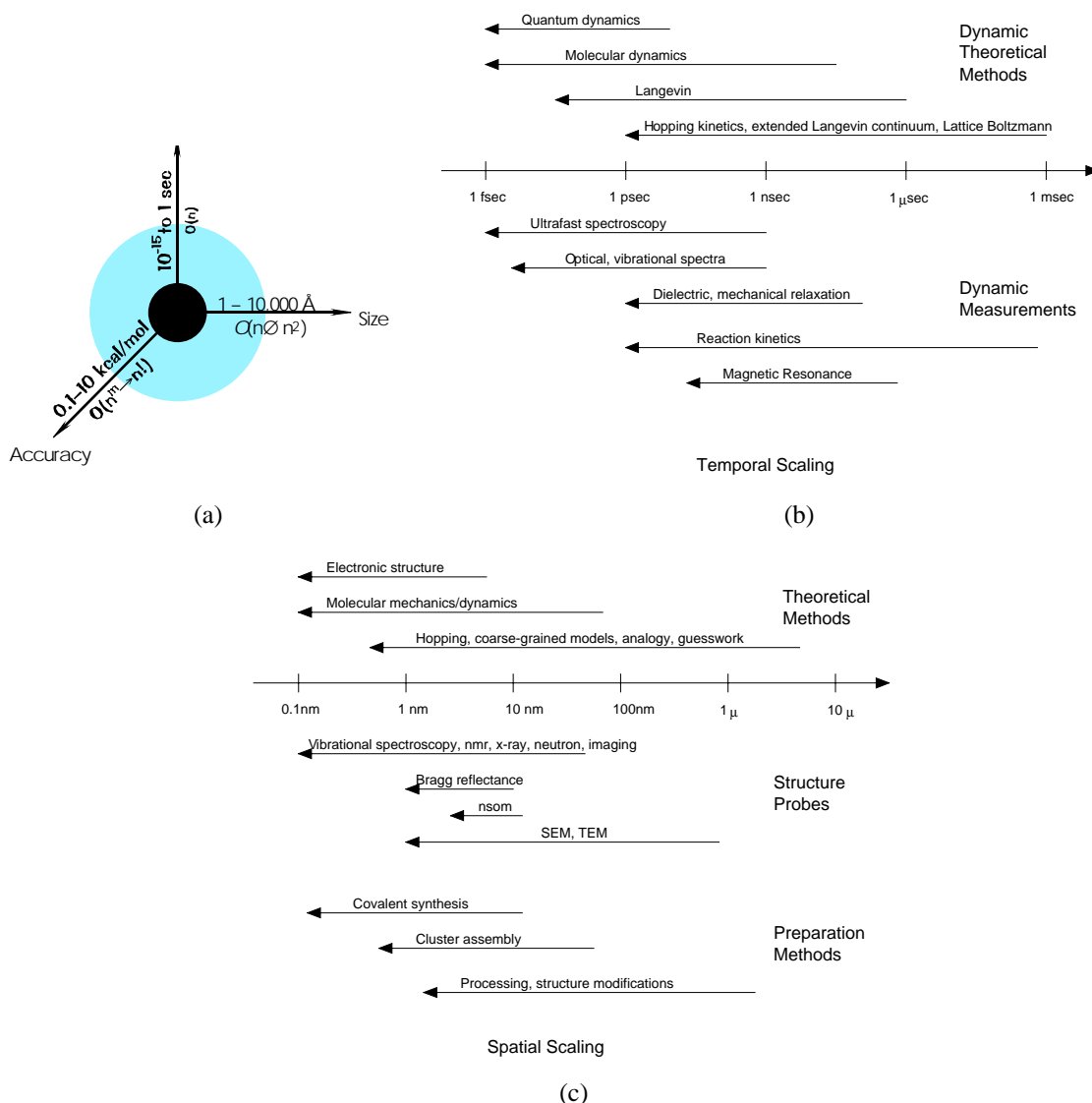

(a)

(b)

(c)

Figure 2.1. Scales and scaling of computational complexity for molecular calculations on nanoparticles.

Whereas molecular dynamics simulations can be successfully used to examine local, relatively short-time-scale motions, this approach is limited on the full scale of relevant motions. Since relaxation times in condensed phase materials such as polymeric systems extend from picoseconds to hours, many of the important questions are simply not susceptible to classical molecular dynamics. As an alternative, one can turn to a coarser scale, considering Brownian-like motion such as described by Langevin dynamics. It is clear that progress in the area of nanoparticles demands that multiple theoretical approaches be brought to bear on single problems, and that diverse approaches be

encouraged. At the same time, there remain opportunities for advancing relatively established methods to improve access to larger systems and longer times. Examples include the development and implementation of methods with linear size scaling in quantum chemistry and methods with multiple time steps and approximations for evaluation of long-range forces in molecular dynamics.

2.7.2 Nanoscale Lubrication

Contact person: P. Cummings, University of Tennessee

A common feature of nanoscale mechanical devices is their need for lubrication between moving surfaces separated by nanometer-sized gaps. For example, the operation of a magnetic recording device relies on the relative motion of the magnetic head and the recording media with a spacing on the scale of nanometers, producing shear in the fluid between the surfaces. The need to achieve higher linear recording density and thus high data storage is pushing this spacing to less than 25 nm, typically using a non-Newtonian liquid-bearing interface to achieve low friction during high speed operation. Common liquid lubricants are perfluoropolyethers, whose steady-state shear rate is as high as $\sim 10^8$ s^{-1}, with extremes of up to two orders of magnitude higher, well beyond the range of strain rates accessible to current experimental characterization methods. Similar shear rates arise in the lubrication of many microelectromechanical systems (MEMS), including micromotors.

In recent years, surface force apparatus (SFA) experiments on model lubricants, including alkanes, have provided intriguing insight into nanoscale lubrication, suggesting that the viscosity of confined nanoscale lubricant films is orders of magnitude higher than that of the same bulk lubricant, and that the nano-confined lubricants are non-Newtonian (shear-thinning) over ranges of strain rate (10^2-10^5 s^{-1}) for which the corresponding bulk lubricant is Newtonian. This has raised questions about the feasibility of lubricating MEMS devices and concerns that high power consumption (relative to size) will be required to overcome friction at start-up and viscous resistances during operation. Careful molecular dynamics simulations at high strain rates ($\sim 10^8$ s^{-1} and higher) have shown little difference between confined and bulk behavior (Figure 2.2 and Figure 2.3).
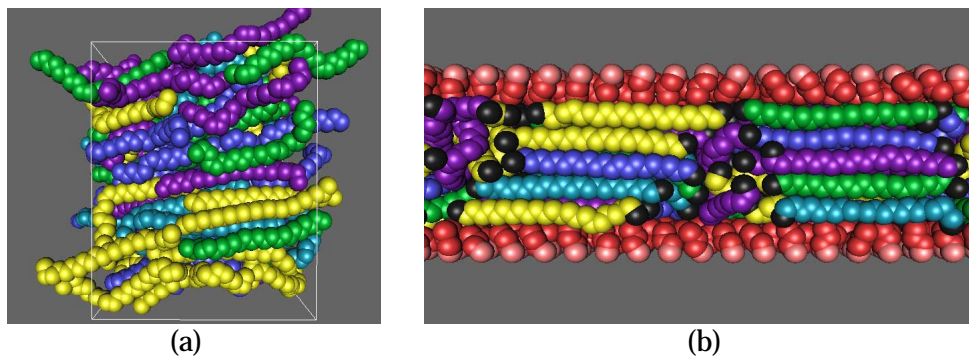

(a)   (b)

Figure 2.2.   (a) Snapshot of n-tetracosane in bulk under shear flow at a shear rate of 7 x 10^9 s^{-1}, density of 0.82 g cm^{-3} and temperature of 313 K. Only the carbons are shown. Molecules are shaded in different colors to aid in distinguishing them. (b) Snapshot of n-tetracosane under shear flow confined between two walls with tethered butane chains, with wall spacing of 3.6 nm, the same apparent shear rate, core liquid density of 0.82 g cm^{-3}, and temperature of 313 K. End groups are shown in black.
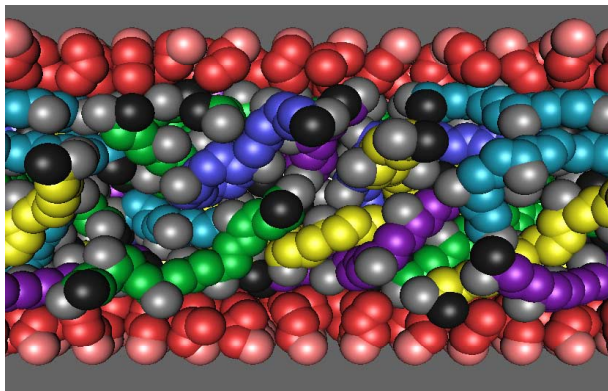
Figure 2.3.   Snapshot of squalane under shear flow confined between two walls with tethered butane chains, with wall spacing of 3.6 nm, the same apparent shear rate as in Figure 2.2, core liquid density of 0.82 g cm^{-3}, and temperature of 323 K. Sidegroups are shown in gray.

However, there is a fundamental disconnect between the strain rates accessible to molecular simulation (~10^8 s^{-1} and higher) and to experiment (~10^5 s^{-1} and lower). The disconnect can only be bridged by much larger scale molecular dynamics calculations on future massively parallel supercomputers permitting accurate simulations at lower strain rates and extensions of the SFA experiments to higher strain rates. A similar problem occurs on simulations of glasses in terms of reaching the glassification temperature.

2.7.3   Simulations of Carbon Nanotubes

Contact person: M. Meyyappan, NASA Ames

Carbon nanotubes (CNT) exhibit extraordinary electronic and mechanical properties. In the past few years, simulations have been valuable to compute the properties of CNT, evaluate potential applications, and design interconnects, sensors, and functional devices. The electronic structure of CNT can be either metallic or semiconducting depending on both the diameter and chirality of the tube. The possibility of connecting nanotubes of different diameter and chirality has the potential to create heterojunctions leading to functional electronic devices, logic gates and circuits. Figure 2.4 (Menon and Srivastava 1997) shows formation of a metal-semiconductor-metal T junction using (5, 5), (10, 0), and (5, 5) nanotubes. This structure was optimized using a generalized tight-binding molecular dynamics scheme.

Molecular machines in the simplest form of molecular bearings, shaft and gear, and multiple gear systems are of interest since they can lead to functional nanoelectromechanical systems (NEMS). Figure 2.5 shows a carbon nanotube-based gear, which is 2 nm in diameter. Shafts are single-walled carbon nanotubes and gear teeth are benzyne molecules bonded onto the nanotube. This is a simple, synthetically accessible structure. Molecular dynamics simulations were used to investigate the properties and design space of the CNT gears.
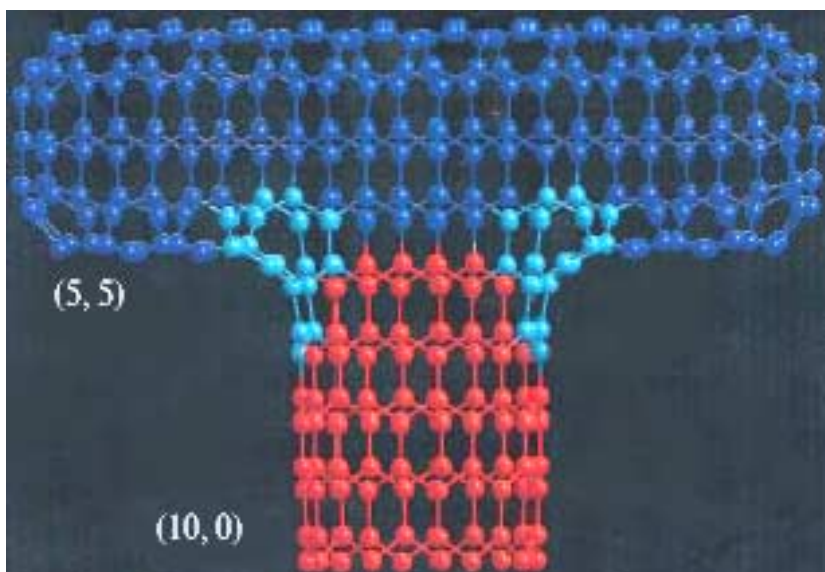
Figure 2.4.   Metal-semiconductor-metal T junction using (5, 5), (10, 0), and (5, 5) nanotubes. The turquoise colored balls denote the atoms forming the heptagons (Menon and Srivastava 1997).
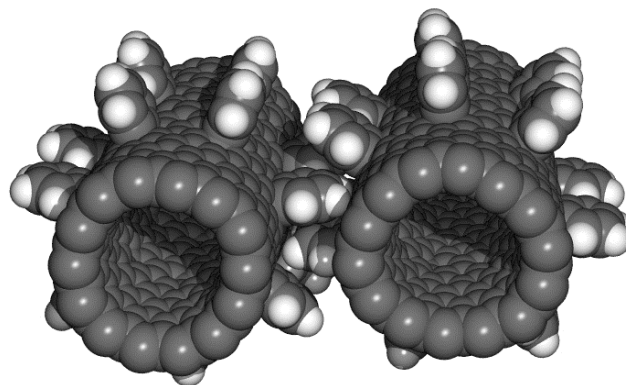

Figure 2.5.   Carbon nanotube-based gears with benzyne teeth (Han et al. 1997; reproduced by permission).

2.7.4   Simulation of Quantum Dots

Contact person: K. Hess, University of Illinois, Urbana

The quantum dot will be a basic element of future devices. The quantum dot can be considered as a large atom. For a small number of electrons, one can use quantum Monte Carlo methods and for larger systems, one can use some form of electronic structure theory, for example, density functional theory (DFT). Figure 2.6 shows an atomistic SiO_2 quantum dot bridging between two silicon surfaces. It is meant to symbolize the connection of nanoelectronics to conventional (silicon—silicon dioxide—silicon) electronics as well as the multiscale nature of the problems (quantum dot connected to bulk). Calculations on this system have been carried out at the DFT level.
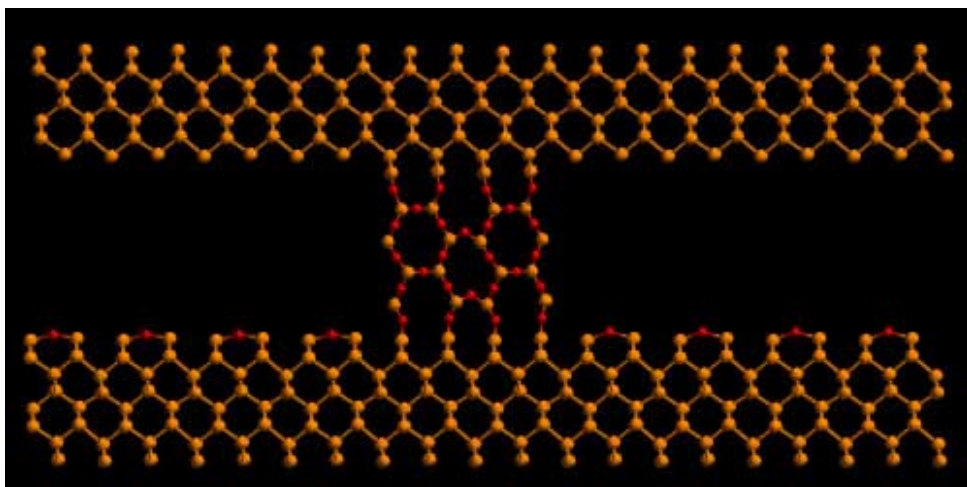
Figure 2.6.   An atomistic SiO$_2$ quantum dot bridging between two silicon surfaces.

2.7.5   Molecular Simulation of DNA Molecule Dynamics

Contact person: Tamar Schlick, New York University

The study of DNA supercoiling—the large-scale folding of the DNA double helix upon itself—is of wide interest because supercoiled DNA is a key functional form of DNA in the cell, directing and facilitating many fundamental biological processes such as replication, recombination, and transcription (Schlick 1995). The problems involved also have practical significance because an improved understanding of the topological and geometric aspects of DNA supercoiling can impact the design of vectors for gene therapy and of topoisomerase inhibitors that act as anticancer or antibacterial drugs.

Kinetic aspects of DNA supercoiling are difficult to measure experimentally on short timescales, and thus simulations can shed insights into the processes and mechanisms involved. The influence of superhelicity on the specific problem of site juxtaposition was studied using a macroscopic wormlike chain/bead model of DNA that considers thousands of base pairs (the DNA diameter is around 2 nm and the length when stretched is 340 nm per 1,000 base pairs) in combination with an efficient Brownian dynamics algorithm. The potential energy accounts for bending and torsional deformations, screened electrostatic terms, and hydrodynamic interactions. This combination makes possible simulations over millisecond time frames that account for key factors that affect DNA conformational flexibility. Previously impossible measurements can be made regarding time estimates for site juxtaposition. Site juxtaposition is the process of bringing linearly distant DNA segments together in space due to the internal dynamics of the DNA molecule. Based on analyses of trajectories such as shown in Figure 2.7 for 3,000 base pairs, the site juxtaposition times can be determined as a function of the superhelicity, the salt concentration, and the separation distance between the sites. These measurements help in the analysis of site-specific recombination reactions to provide lower time bounds for site synapsis (Jian et al. 1998).
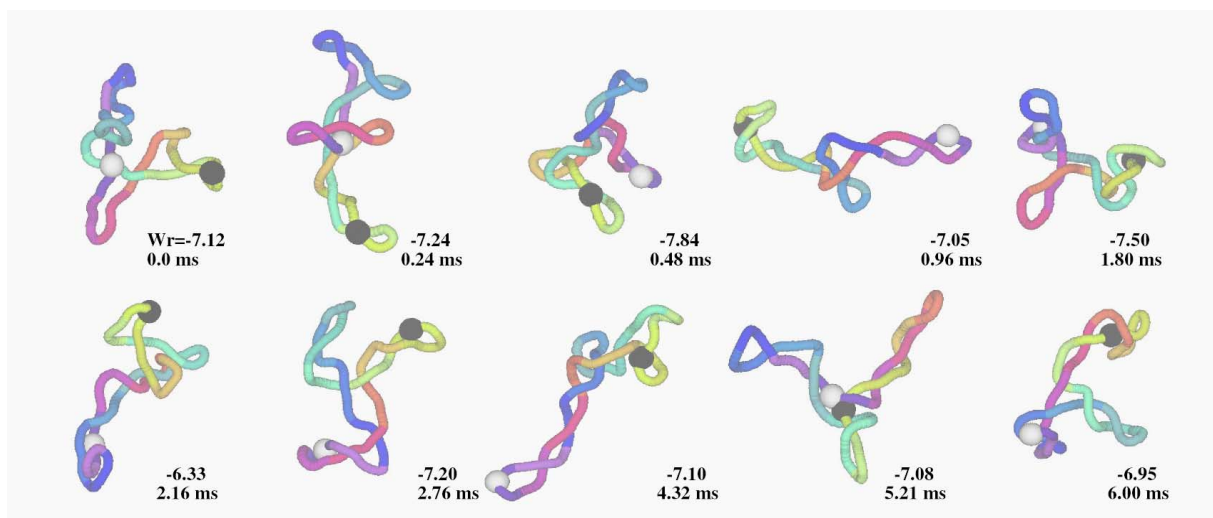
Figure 2.7.   Brownian dynamics snapshots of DNA: Brownian dynamics snapshots of 3,000 base pairs of circular DNA focusing on the juxtaposition of two segments separated by 1,200 base pairs over 6 ms, showing the large random motions that bring sites together (figure prepared by Jing Huang).

Mechanistic details of the dynamic process could also be inferred. Current studies involve extensions to DNA systems of size 12,000 base pairs, and planned work involves incorporation of DNA sequence effects.

2.7.6   Simulation of quantum confinement in silicon nanocrystals

Contact person: J. Chelikowsky, University of Minnesota

Naturally occurring silicon has a low radiative efficiency in the optical region. For this reason, although silicon is the material of choice for making electronic devices, it is not a good material for making optical devices such as solar cells and lasers. Its optical gap is too small. This is in contrast to other semiconductors like gallium arsenide, which has a larger optical gap. As a consequence, gallium arsenide is a material of choice for lasers and other optical applications. If the properties of silicon could be altered to resemble gallium arsenide, then one would have a universal material for building all opto-electronic devices. This is an important consideration, as a huge investment has been made in processing and manufacturing silicon-based devices.

Recently, it has been discovered that the optical properties of silicon can be altered by confining the optical excitation to a small region of space, e.g., within a large cluster of silicon atoms. These large clusters are called quantum dots. The dots are fragments of crystalline silicon that have been terminated by a passivating material such as atomic hydrogen. Such a quantum dot is illustrated in Figure 2.8. Its optical gap measured as function of dot size is illustrated in Figure 2.9. The optical excitation for the quantum dot is significantly enhanced, both in frequency and in intensity. This effect, called quantum confinement, makes silicon resemble gallium arsenide in terms of its optical properties. For example, the excitation energy for the silicon dots in Figure 2.9 is as large as 2-2.5 eV, twice the optical gap of crystalline silicon, and comparable to the gap of 1.5 eV in gallium arsenide. First principles, parameter-free calculations for the optical gap in silicon quantum dots have been performed to verify the role of quantum confinement and

to assess the experimental interpretation. Using massively parallel computer platforms and newly developed algorithms to examine such large systems, clusters up to 30 Å in diameter can be handled.

The largest cluster considered was $Si_{575}H_{276}$ (Figure 2.8). This dot contains several thousand electrons; consequently, the change in energy upon absorption of light is very small relative to the total energy of the electrons. By focusing only on the role of the electronically active states, this calculation becomes tractable. This is the first time optical excitations have been computed for a dot of this size. In Figure 2.10, the calculated optical gaps are compared to experiment. The overall agreement is quite good. This work has led to a better understanding of the role of quantum confinement and a means of predicting optical transitions in nanostructured matter.
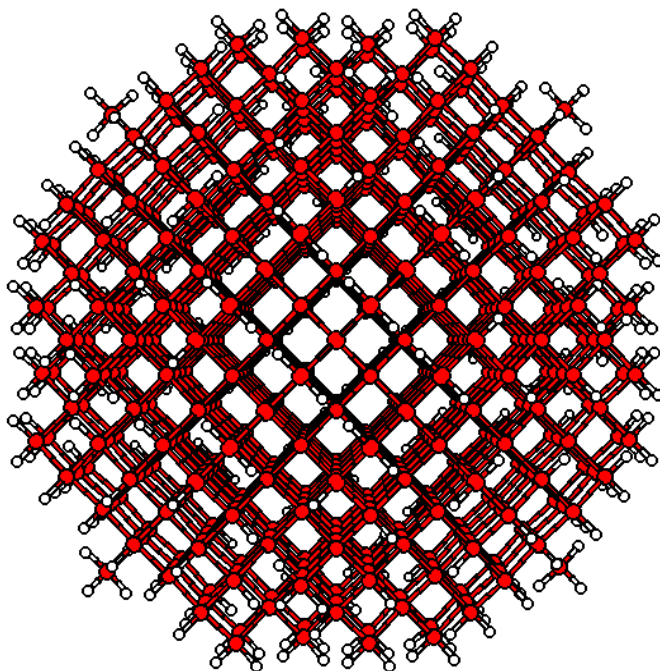

Figure 2.8.   Ball and stick model of $Si_{575}H_{276}$. The white dots correspond to H atoms, which passivate the surface of the dot.

2.7.7   Molecular Dynamics Simulation of Piezoelectric Polymers
Contact person: Jeffrey Hinkley, NASA Langley Research Center

Researchers at NASA Langley Research Center (LARC) have simulated the molecular motion during poling of an amorphous polyimide. The approach involved parameterizing interatomic forces and atomic charges using quantum mechanics, verifying against experimental measurements of density and dipole moment, and predicting dipolar response to an electric field and the dielectric relaxation strength. Based on insights from this simulation, dozens of proposed new polymers have been rapidly screened, saving considerable effort in the laboratory. Similar methods can be applied to calculations of solubility, interactions with surfaces (adhesion), and permeability to gases such as hydrogen propellant.
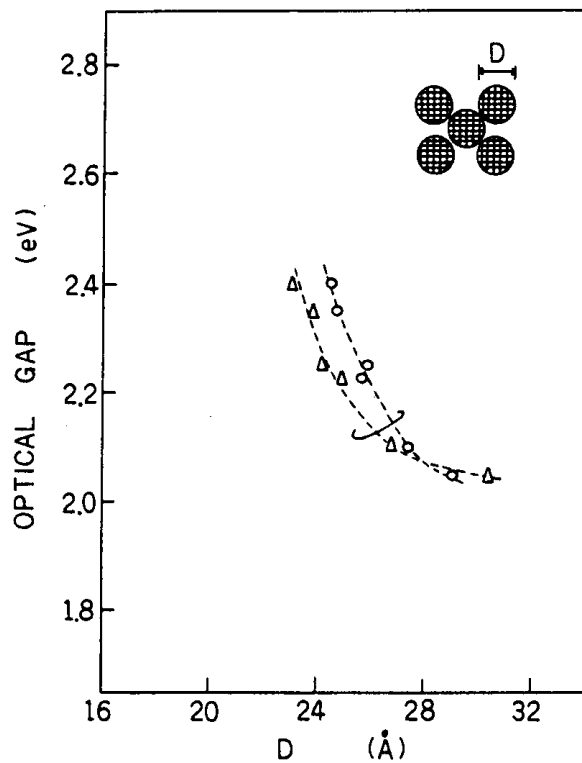
Figure 2.9. Experimental optical gaps for silicon quantum dots. D is the diameter of the dot. The results are from Furukawa and Miyasoto (1988). The two sets of experimental data represent different estimates for the size of the dots.
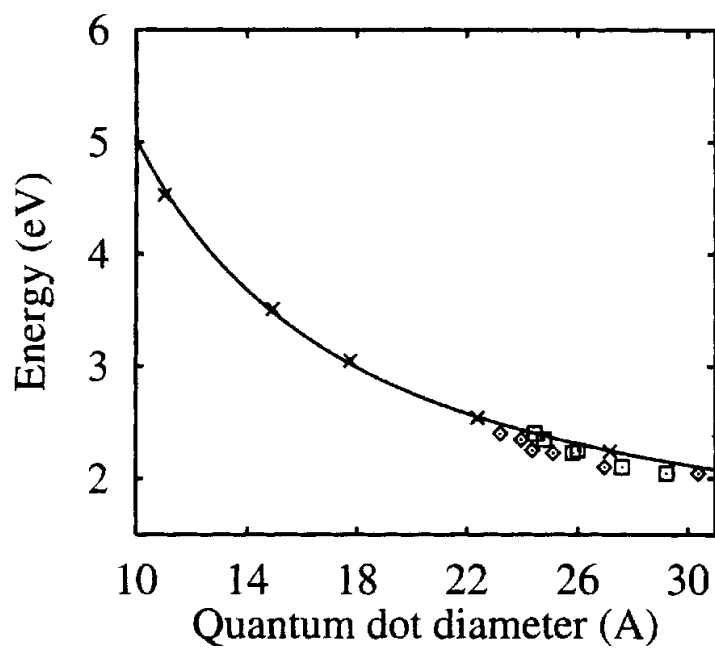

Figure 2.10. Theoretical optical gaps versus experiment. The theory (solid line) is from Ogut, Chelikowsky, and Louie (1997). The open symbols are from experiment; see Figure 2.9.

The simulation shown in Figure 2.11 is used for lightweight sensors for integrated smart materials. In this case, the breakthrough is observation of piezo activity up to 100°C above temperature limits of state-of-the-art materials. Future directions include simulation of semicrystalline materials, nanocomposites containing layered silicates, and revolutionary organic/inorganic hybrids.
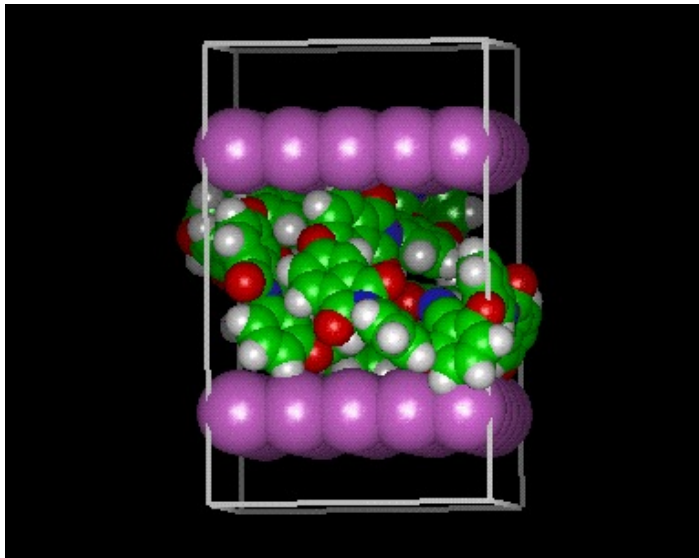

Figure 2.11. An amorphous cell at experimental density containing 5 repeat units of a piezoelectric polyimide. Planes of large spheres represent metal electrodes; they are used to simulate a poling field.

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