A Visual Approach to Nanotechnology Education*

CHARLES XIE

The Advanced Educational Modeling Laboratory, The Concord Consortium, Concord, MA 01742, USA. E-mail: qxie@concord.org

HEE-SUN LEE

Department of Physics, University of California Santa Cruz, Santa Cruz, CA 95064, USA. E-mail: hlee58@ucsc.edu

This paper presents a systematic visual approach to teaching concepts in nanotechnology. Five types of mathematical models are used to generate visual, interactive simulations that provide a powerful software environment for virtual experimentation. The nanotechnology content areas covered by this approach are discussed. A variety of instructional strategies for effective use of these simulations are discussed. Preliminary results from a pilot study at the college level demonstrated the potential of this approach for improving nanotechnology learning.

Keywords: nanoscience; nanotechnology; computer simulation; scientific visualization; science education; knowledge integration

1. Introduction

Nanotechnology is a rapidly growing field. Technologies that are 'hot' today may fade away tomorrow. But the foundational concepts are not as volatile. This paper focuses on teaching basic concepts of nanotechnology, which take root in physical and biological sciences and expand into exciting visions such as atomically precise manufacturing [1, 2].

A solid foundation is critically important to students, who must be prepared with universally applicable knowledge and skills needed to understand various technologies and applications that are constantly being proposed and invented. Disseminating the grand visions of nanotechnology to students is equally important, as among them there are future generations of scientists, engineers, and technicians who will help realize and advance the visions.

Teaching nanotechnology concepts is not a trivial task, however. A large part of the foundation for nanotechnology is the basic science about electrons, atoms, and molecules. None of these microscopic objects behave like anything students see and experience in everyday life. A deep understanding of nanoscience builds upon thermodynamics, statistical mechanics, and quantum mechanics [3]. These subjects often pose learning difficulties to students.

This paper presents a visual approach to tackle these issues for a broad audience in K-16 education. Many nanotechnology experiments are still infeasible to carry out in the classroom. But they can be simulated on the computer. Revolutionary ideas such as nanomachines and nanofactories are something that does not exist yet. But they can be conceived and simulated, too, based on known scientific principles. In fact, this is the approach taken by Drexler in his foundational book that popularized the concept of nanotechnology [4]. In the book, he predicted molecular machines based on computer simulation. Unlike his theoretical analysis that only a limited number of students can follow, the visual simulations of hypothetical nanomachines described in this paper present those ideas in a more accessible form.

This work is based on the *Molecular Workbench* (MW) software (http://mw.concord.org) developed by the first author [5]. The software simulates the dynamics of electrons, atoms, and molecules that dominate the nanoscopic world. As the computational engines of MW grew out of contemporary molecular modeling research [6], MW simulations generate excellent digital representations of nanoscale phenomena. With its graphical user interfaces, the MW environment provides a virtual laboratory in which simulated nanoscale processes can be examined and manipulated on the computer screen in real time. This simulation capacity offers a powerful means of experiential learning in the field of nanotechnology that has even been applied at the elementary school level [7]. This paper will present the five mathematical models for modeling nanosystems in MW and summarize the nanotechnology content that can be taught using them. Various instructional strategies for using simulations in different settings will be discussed and compared. Preliminary data based on a pilot study at the college level will also be presented.

2. Mathematical models for nanosystems

An early visionary of nanotechnology [8], physicist Richard Feynman once said, 'If, in some cataclysm, all of scientific knowledge were to be destroyed, and only one sentence passed on to the next generations of creatures, what statement would contain the

most information in the fewest words? I believe it is the atomic hypothesis . . . that all things are made of atoms—little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another. In that one sentence, you will see, there is an enormous amount of information about the world, if just a little imagination and thinking are applied' [9].

The enormous amount of information in Feynman's one sentence is precisely what molecular dynamics delivers. Classical molecular dynamics is a computational method that simulates the movements of atoms and molecules by numerically solving Newton's equation of motion according to their interactions [10]. With interactive computer graphics that visualizes and controls molecular dynamics and provides an assistive imagination and thinking tool, Feynman's insight can be shared among students.

Four types of 2D or 3D molecular dynamics models are available in MW for simulating nanosystems at different levels of details, as briefly discussed below.

2.1 The all-atom molecular dynamics

The all-atom molecular dynamics models every single atom as an independent particle that interacts with one another through the van der Waals force and electrostatic force, and every single molecule as a group of atoms that are connected through bond-stretching, angle-bending, and dihedral torsion forces that approximate the effect of covalent bonding [6]. This model is needed when an accurate description of the chemical structure of a nanosystem is required. For example, the simulations of fullerenes such as carbon nanotubes (Fig. 1), buckyballs, and graphenes generally require this level of details.

2.2 The coarse-grained molecular dynamics

Large nanosystems such as those commonly encountered in molecular biology often involve a tremendous amount of atoms and bonds. All-atom molecular simulations of large nanosystems on a typical computer take too long to be practical for student exploration—the force calculations will be too time-consuming for a simulation to produce enough frames per second to render a smooth animation. Furthermore, two current trends in educational computing prompted us to look for alternative solutions that do not rely on super-computing to come to schools. First, with Moore's Law approaching the limit, traditional desktop computers in schools are not expected to get much faster any time soon. Second, more schools are
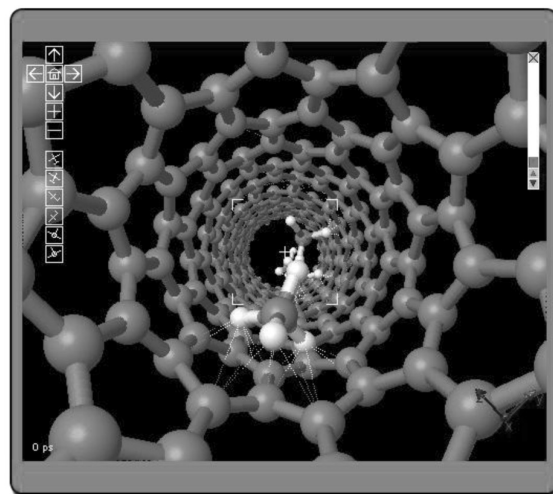

Fig. 1. An all-atom molecular dynamics simulation of motion of methane molecules moving through a carbon nanotube.

adopting tablets that are actually powered by down-graded central processing units.

Coarse-graining provides a possible workaround for the problem. A coarse-grained model greatly reduces the number of degrees of freedom of a system by keeping the most important features and removing the relatively trivial details [11, 12]. Without compromising the qualitative understanding of the idea, a coarse-grained simulation that models large molecules with as few particles ('beads') as possible runs much faster than that for the same system in the all-atom representation.

Figure 2 gives an example of how a highly simplified model can be used to illustrate the main idea of translation from RNA code to a protein. Because of the dramatic simplification, this 2D model can run in real time, permitting students to mutate the RNA code and see how a different protein is synthesized by this molecular machinery.

2.3 The Gay-Berne molecular dynamics

Most coarse-grained models use spherical particles to represent groups of atoms. However, individual spherical particles do not have a rotational degree of freedom and, therefore, cannot show structural transitions in molecular orientation typically observed in mesophases (intermediate states between liquid and solid). The Gay-Berne potential [13] and its extensions [14, 15] provide a coarse-grained model based on elliptical particles. The potential can be used to approximate linear polymers and their interactions when their internal structures are adequately rigid and their intramolecular forces do not have a significant contribution to the overall assembly dynamics (the upper image in Fig. 3). The potential has been widely used to
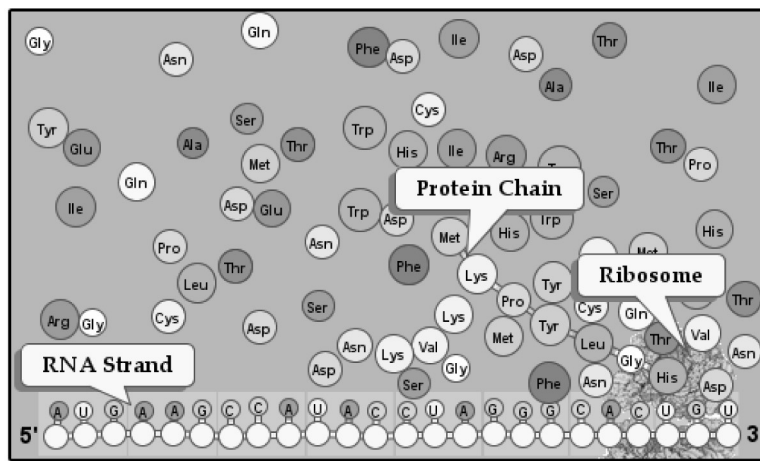
Fig. 2. A coarse-grained dynamics simulation of translation (making proteins from messenger RNA). Each amino acid, RNA base, and RNA backbone are represented by a particle. The amino acids randomly bounce into the ribosome site and the one that matches the current RNA triplet will be attached to the growing polypeptide. The solvent is not explicitly modeled.

simulate liquid crystals and cell membranes. It is capable of showing transitions among nematic, discotic nematic, and biaxial nematic phases [14]. By adding point charges and dipole moments [15], elliptical particles can self-assemble into fairly complex phases and patterns (the lower image in Fig. 3).

2.4 The soft-body dynamics for biomolecules

Illustrations in molecular biology commonly use objects of arbitrary shapes to represent macromolecules. An important objective of our work is to transform these static pictures into interactive simulations that students can not only view but also manipulate.

Most biological macromolecules are soft—they vibrate, react, deform, fold, and assemble. In many cases, it is primarily the molecular surfaces that are important in affecting the intermolecular interactions and dynamics.

Soft body dynamics [16] in MW models a flexible molecular surface as a network of particles connected by elastic constraints. These 'springs' maintain the distances between two neighboring particles, the angles among three adjacent particles, and the dihedral angles linking four adjoining particles. For 2D models, these discrete particles are placed along the edge of an object (the lower image in Fig. 4). For 3D models, these particles are placed on the surface mesh of an object. Physical interactions among soft bodies are enabled by giving these particles properties such as molecular mass, a stiff repulsive core, an attractive force, or an electric charge. This allows many interesting macromolecular phenomena to be modeled, such as self-assembly [7], docking, molecular recognition, and so on.
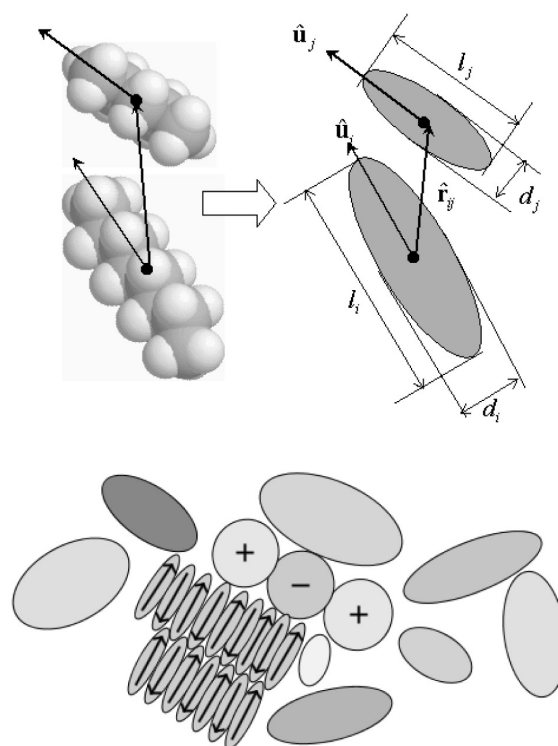

Fig. 3. The Gay-Berne potential provides another coarse-grained model. The '+/−' signs represent point charges, whereas the arrows electrical dipole moments.

2.5 Quantum dynamics

The above mathematical models are based on classical molecular dynamics, which cannot model quantum effects that are significant in the nanoscale world. Quantum mechanics is responsible for novel properties of nanostructures such as nanoparticles, quantum dots, and graphenes. As the nanotechnol-
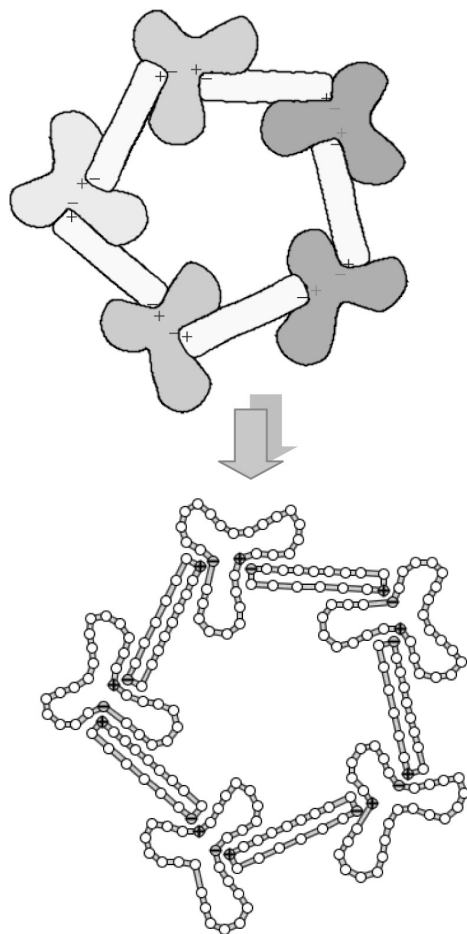
Fig. 4. The mass-spring model is used to discretize 2D soft bodies (the angular constraints are not shown). Given physical properties, the self-assembly of these soft bodies can be simulated.
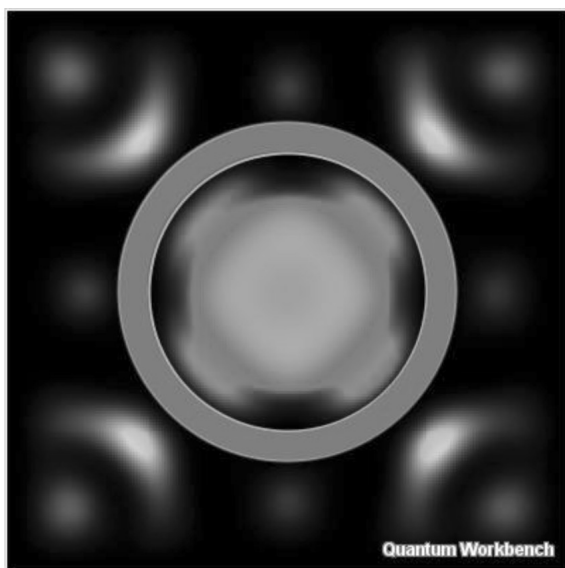

Fig. 5. Quantum dynamics supplements molecular dynamics to provide visualizations for quantum concepts. The image shows a snapshot of the quantum wave in a curricular container with a finite barrier height. The wave is colored by its phase.

ogy pioneer Donald M. Eigler (whose landmark experiment in 1989 proved the feasibility of atomically precise manufacturing for the first time) put, 'we become quantum mechanics—engineering and exploring the properties of quantum states. We are paving the way for the future nanotechnicians' [17].

As supplements to the molecular dynamics models, we have built 1D and 2D quantum mechanics simulation engines for MW. These engines are based on efficient finite-difference time-domain algorithms for solving the time-dependent Schrödinger equation [18]. Fig. 5 shows a 2D simulation of quantum waves contained in a circle with a finite barrier height. The dimmer waves outside the container show the leakage due to quantum tunneling through the barrier.

3. Teaching nanotechnology using visual simulations

The visual simulations powered by the above five mathematical models cover a wide scope of nanotechnology content. It is impossible to present all of them in this paper. The following subsections will showcase a few selected topics in which the visual approach demonstrates its unique strength.

3.1 The basic science about electrons, atoms, and molecules

Fundamental concepts such as atomic structure, chemical bonding, interatomic interactions, and so on are the building blocks of nanoscience and nanotechnology. The visual quantum mechanics and molecular dynamics simulations in MW, to some extent, serve as a set of virtual atomic microscopes for viewing into the nanoscopic world and exploring these concepts.

For example, the interactions among electrons and nuclei determine the chemical properties of atoms and molecules. It is the gain, loss, and sharing of electrons that governs all chemical reactions. A chemical bond is created when two or more atoms share their electrons. The distribution of electrons in atoms and molecules affects how they interact and form various structures and states. Understanding the properties of electrons is a key to understanding chemistry. A quantum mechanical simulation in MW presents a 'reaction chamber' in which students can control the electron dynamics and 'design' the products of a simple chemical reaction (Fig. 6). This simulation uses the Imaginary Time Propagation method for solving the Schrödinger equation [19] to achieve the visual effect that the electron cloud automatically and dynamically seeks the ground state for the configuration the user creates by dragging the mouse.
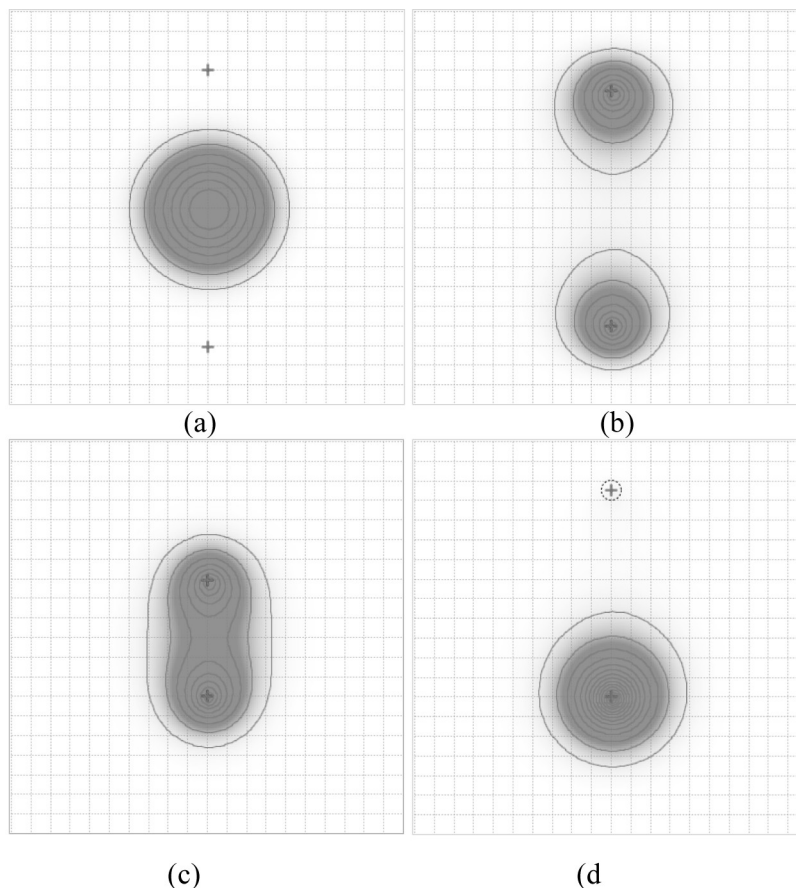
Fig. 6. This interactive simulation allows students to discover possible states of a 2D quantum system. Because the quantum mechanics calculation is done in real time, the shape of the electron cloud (represented by the haze) dynamically responds to the user's drag-and-drop of the protons (represented by the plus signs). (a) The initial state of two protons and an electron cloud. (b) The formation of two hydrogen atoms polarized by each other, showing the origin of the van der Waals force. (c) The formation of a covalent hydrogen molecule when the electron cloud overlaps significantly. (d) The formation of a hydrogen anion and a proton.

3.2 Thermodynamics and statistical mechanics

Thermodynamic effects are inevitable in nanosystems at finite temperature. One of the problems they cause is the positional uncertainty of atoms resulting from constant thermal fluctuations. Therefore, random thermal motion must be considered while engineering nanosystems.

Statistical mechanics studies the thermodynamic properties of materials based on the properties of their constituent particles and the interactions among them. Molecular dynamics provides a powerful tool for teaching the ideas through interactive visualizations.

For instance, students have long been taught that temperature is defined as the average kinetic energy of the particles in the system. But they are rarely asked why that is a good definition. The explanation lies deeply in the heart of statistical mechanics. Fig. 7 shows two molecular dynamics simulations we have designed to visualize this question. The first

simulation illustrates that different chemical components of an equilibrium system have identical average kinetic energy (Fig. 7a). The second illustrates that the average kinetic energy is approximately the same everywhere for any subset of particles in a container that has reached thermal equilibrium (Fig. 7b). It is the agreement of these statistical properties of average kinetic energy with what we feel about temperature at the macroscopic level that warrants the statistical mechanics definition of temperature. These insights, which are probably not easy to convey without resorting to high level mathematics, can now be delivered through visual simulations such as those shown in Fig. 7.

3.3 Nanoelectronics

Nanoelectronics is an important branch of nanotechnology that holds the promise of making even more powerful computers in the future. The study of
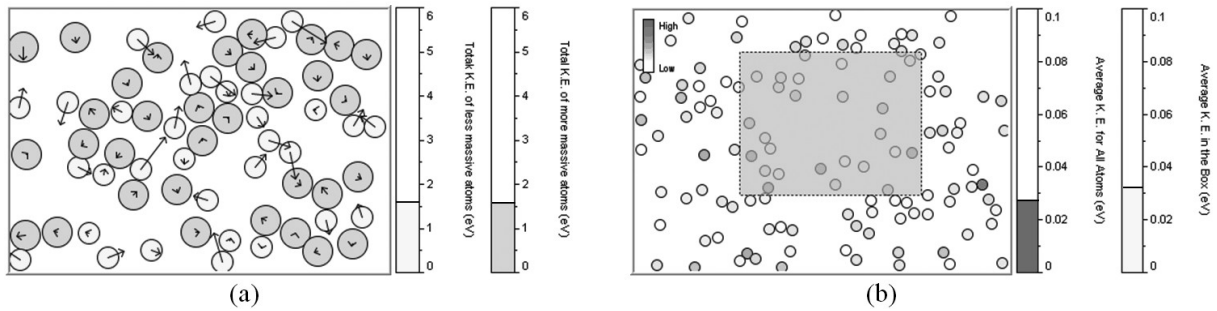
Fig. 7. Two molecular dynamics simulations that show why the average kinetic energy is a good measurement of temperature. (a) This simulation shows that the average kinetic energies of two different types of particles adequately mixed in an equilibrium system are statistically identical. (b) This simulation shows that the average kinetic energy of the particles inside the selected rectangle, regardless of its size and location, is statistically equal to that of all the particles. In both cases, the bar graphs display the average kinetic energies of the compared sets calculated by the molecular dynamics simulations.

transistors is central in nanoelectronics. The junction field-effect transistor (JFET) is the simplest type of field-effect transistor. Electrons flow through a semiconducting channel between source and drain terminals. By applying a bias voltage to a gate terminal, the channel is pinched, so that the electric current is impeded or switched off completely.

This phenomenon can be simulated using either the classical dynamics or the quantum dynamics method available in MW. The classical dynamics simulation shows the particle view of electron flow (Fig. 8a), whereas the quantum dynamics simulation presents a wave view of quantum transport

(Fig. 8b). Both views can explain the mechanism of a transistor. But acute readers may notice that in the quantum simulation there is a weak tunneling current even if the transistor is in the off state—something that does not happen in a classical simulation.

3.4 Virtual nanotechnology experiments and nanosystem designs

We have developed simulations for teaching scanning tunneling microscopy [20], electrostatic self-assembly [21], and atomic layer deposition [22]. These simulations can supplement lecture or labora-
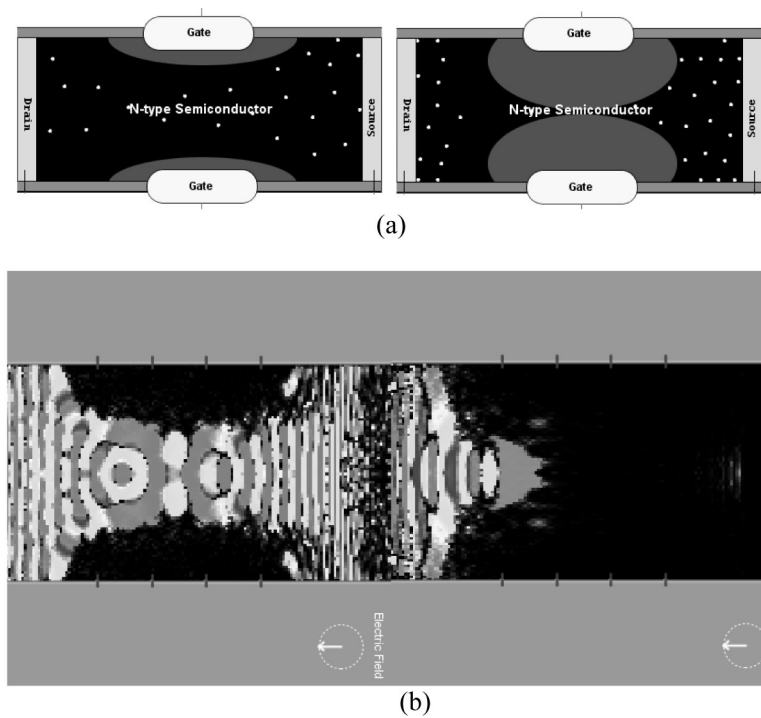

Fig. 8. (a) A classical molecular dynamics simulation of a JFET. The small white dots represent electrons. (b) A quantum dynamics simulation of a JFET. The electron wave is colored by its phase. In both simulations, students can adjust the gate voltage to switch the transistor on (the left images) and off (the right images).

tory with additional opportunities of learning. The interactivity design of some of these virtual experiments even simulates laboratory procedures. In technician education, connecting the underlying scientific principles with laboratory manipulations is desirable as it helps students develop a deeper understanding of a procedure or a protocol. The science knowledge can generally improve their skills in troubleshooting and quality control.

As pointed out in the Introduction section, nanotechnology education should not just teach fundamentals. Perhaps more importantly, it should also pass the bigger picture of nanotechnology to students. Futuristic nanosystems, such as those conceptual nanomachines envisioned in Drexler's foundational book [4], can be brought to the classroom through simulations to provide inspirations. We have created a collection of fictitious nanomachines such as nanogears and nano conveyor belts (Fig. 9). Although these hypothetical nanomachines have not been chemically synthesized, they can still be used as some kind of serious 'science fiction' to stimulate students' interest just like Drexler's sketches did for scientists.

As MW also empowers users to create simulations, students can be challenged to modify or invent new nanomachines to do some desired work. Because it is based on the Newtonian mechanics, molecular dynamics provides a way to design mechanosynthesis, in which reactive molecules would be brought together in planned sequences, positions, and orientations by mechanical forces. This kind of design activities could open many opportunities of inquiry for students to learn more deeply and more broadly [23]. Virtual nanomachine design could one day become an important activity for learning nanotechnology, equivalent to today's popular student activities that engage them to learn Newtonian mechanics by designing impressive animations of mechanical systems [24].

4. Instructional strategies using visual simulations

Interactive, visual simulations are often attractive presentations to teachers and students [25–30]. However, the attraction in the first impression is not a guarantee of learning. Research has identified a problem called 'deceptive clarity': While students overwhelmingly favor visualizations, they may learn superficially [31]. Complex simulations like the ones shown in this paper sometimes contain an enormous amount of fleeting details. Some guidance is needed to realize their teaching potential. Classroom dynamics, such as teacher-student interaction and student-student collaboration [32, 33], can play a positive role on amplifying the power of visual simulations. For instance, asking students to elucidate what they see from visualizations helps them realize what they do not actually understand and can spur them to revisit the visualizations to remedy gaps in their knowledge. A recent study in education and cognitive development suggests that explaining plays a key role in learning and generalization: When learners explicate, they learn more effectively and generalize more readily [34].

There are many different ways of using visual simulations in the classroom. Each has its own usefulness. A traffic analogy, in which a simulation is metaphorized as a transportation vehicle, may be a good agency for explaining them.

4.1 Using simulations to assist lecture

Teachers can use visual simulations in the classroom to enrich their lecture. A visual simulation can be projected onto a screen and shown to the whole class. From this point on, there are two ways of taking advantage of the simulation:

(1) 'Students as passengers in a taxi cab': The teacher shows students a simulation and tells
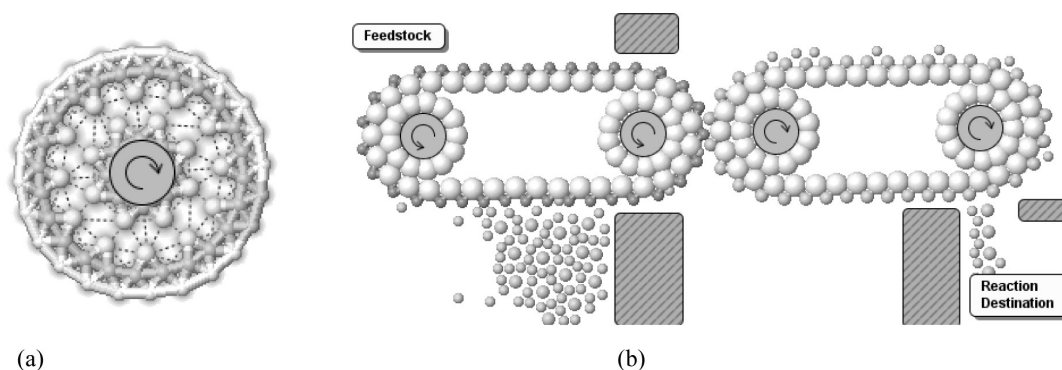

(a)																	(b)

Fig. 9. (a) An internal nanogear that resembles Fig. 1.1 in Drexler's defining book about nanosystems. The dashed lines show the van der Waals interactions that facilitate the 'transmission' mechanism. (b) Two nano conveyor belts that actively sort and transport a certain type of feedstock molecules, resembling Fig. 13.7a in Drexler's book. The nanoscale mechanisms in both (a) and (b) are fictitious.

them what the result means at the end. The teacher's role is to 'drive' students to the destination set by the learning goal. Students may remember the 'destination' knowledge but less about the dots along the path that connect to it because they just passively watch the teacher's demonstration of the simulation. This is a typical use of simulations when the teacher does not have enough time or the intermediate details are not important to the lesson.

(2) 'Students as tourists in a bus': The teacher shows students a simulation but makes 'frequent stops' to prompt students to notice the details and think about them. At each pause, the teacher may ask students to predict what will happen or explain what they observed. Students can also suggest an input or change to the simulation that the teacher will implement in front of the class. Changing the course of the simulation may lead to new questions and new inquiries. In this scenario, the interactions between the teacher and the students are mediated by these interaction opportunities provided by the simulation. In some cases, this mediation can be used to make a 'screenplay' that scaffolds effective lecture.

4.2 Using simulations as virtual experiments

If enough computers are available and time permits, students should be given opportunities to interact with simulations themselves just like in a hands-on laboratory. In this case, students are encouraged to explore, but the tension between student autonomy and their need for guidance needs to be addressed. Research has shown that guided inquiry can be more effective than open inquiry [35]. Guided inquiry uses clear goals, careful scaffolding, ongoing assessment, and teacher intervention to lead students to independent learning. Dynamic visualizations often require specific guidance regarding search strategies and targets that will lead to the construction of a satisfactory mental picture [30]. We recommend two strategies for guided inquiry using visual simulations:

(1) 'Students as drivers with a GPS guide': Students work with a simulation individually or in groups under a set of instructions that gradually lead them to the answers. This scaffolded approach sets a 'sandbox' that constrains student exploration within, which allows their progression to be more tightly linked to the learning goals. Some flexibility in the instructional design may allow students to sidetrack, but they are always guided back to the main learning route by just-in-time intervention from the teacher or the intelligent tutor built into the simulation. In fact, this has been the design principle for many of the existing learning modules we developed using MW.

(2) 'Students as drivers with a map': Students work with a simulation tool individually or in pairs. They are given clear learning goals and prepared with the basic knowledge (just like a map that gives a rough idea about cities and streets). But they have to plan their own routes. They figure out the answers or the solutions and thus construct their knowledge [36]. They learn from making mistakes and correcting them, too. Students will need more time on finding the paths and probably detouring in the tasks. There is also a risk that they may not attain the learning goal. The most constructivist version of this approach is to challenge students to design simulations that answer a question or solve a problem [37].

5. Results from a pilot study

Although the ideas of nanotechnology have been infused into many existing courses in science and engineering [38], nanotechnology is not currently taught as an independent course in many schools and colleges. Large-scale educational research dedicated to nanotechnology education is difficult at present time because a large amount of funding is typically needed to recruit and train enough numbers of teachers and students for such a study to take place.

We have conducted a small pilot study in an introductory solid state physics course offered by the Physics Department at the University of California, Santa Cruz. The course objectives included the understanding of fundamental quantum mechanical principles governing the semiconductor physics and the understanding of physical principles behind the building blocks of modern electronic devices, which are related to nanotechnology and can be supported by our visual approach. Although the pilot study focused more on investigating the effect of visualizations embedded in standalone curriculum modules than on a particular nanotechnology topic, the results may be general enough to shed light on how nanotechnology education can benefit from this visual approach.

The solid state physics course consisted of twenty 90-minute long lectures and lasted 10 weeks over a single quarter. Twenty-two sophomores to seniors were enrolled in the class. Among these students, 10 % were female. A demographic survey administered at the beginning of the course indicates uneven prior course backgrounds among the students: 100% had taken introductory physics; 74% had taken thermal physics, 95% had taken introductory modern phy-

sics, 42% had taken electricity and magnetism, 21% had taken quantum physics, and 16% had taken solid state physics.

Due to the fast pace of the course and the vast amount of materials needed to be covered, the instructor used three online MW modules as homework assignments so that individual students could gain more robust understanding of fundamental concepts related to semiconductor devices. The three MW modules were Quantum Basics (QB), Quantum Tunneling (QT), and Semiconductors (SC). The QB module covers probability waves, diffraction and interference, tunneling, bound states, and excited states [39]. The QT module covers factors that affect tunneling, tunneling leakage in computer chips, tunnel injection and release, and nanopore DNA sequencing [40]. The SC module covers thermal excitation, intrinsic and doped semiconductors, electron holes, P-N junctions, and the energy band theory [41]. The instructional design of the three modules was based on the 'students-as-drivers-with-a-GPS-guide' approach. All the core concepts are delivered through one or more visual, interactive simulations that allow students to explore the relationships among properties of various quantum and solid state systems. Each module consists of several inquiry-based investigations in which students experiment with simulations to answer questions addressing the core concepts. Students' answers to the prompts embedded in the modules are collected through the Internet. Table 1 lists the number of visualizations, the number of investigations embedded, the number of prompts, and the implemented time during the course in the pilot study.

In order to investigate the impact of these modules on student learning, a pre/post research design was applied. We administered an identical paper-and-pencil test in the first and the last class of the course in which the three MW modules were implemented as homework assignments. The test consisted of 12 multiple choice items followed by open-ended items that asked students to explain their multiple-choice answers. The items addressed basic concepts related to quantum mechanics (e.g., tunneling, wave functions, and electron behavior) and solid state physics (e.g., metals, semiconduc-

tors, transistors, and P-N junctions). Since the study lacked a control group, we used an indicator of fidelity of implementation that can reflect the amount of students' cognitive engagement with the three MW modules [42]. The impact of the intervention on student learning outcome can be strengthened if students with higher fidelity of implementation change from pretest to posttest to a greater extent than those with lower fidelity of implementation [43, 44]. In this study, we used student answers to all of the prompts embedded in the three MW modules to create an indicator of fidelity of implementation. Nineteen students took the pretest while 15 took the posttest. The QB module was completed by 20 students, the QT module by 22 students, and the SC module by 18 students. In order to account for student learning with the course, we also collected students' course grades provided by the instructor.

The multiple-choice items in the pretest and the posttest were scored dichotomously, i.e. a score of '1' for correct answers and a score of '0' for incorrect or blank answers. The open-ended explanations were scored from 0 to 4 using the Knowledge Integration (KI) Scoring Method [45, 46]. The method is based on the Knowledge Integration Theory [47, 48] that describes students' science learning as eliciting their ideas, adding new scientific ideas, and making connections among the scientifically relevant and meaningful ideas in explaining phenomena or justifying claims [49]. The KI Scoring Method assigns higher scores to students' understanding based on a multiple set of scientifically relevant ideas than those based on a single idea or those based on scientifically non-normative ideas (see Table 2 for a rubric based on the KI Scoring Method for an item related to a semiconductor question shown in Fig. 10). The higher the KI score, the more integrated the student's understanding. The KI assessment method has been validated in multiple field studies involving more than 18,000 middle and high school students in physical, biological, and earth sciences [45, 46, 49–51]. In a four year study [51], the reliability of the KI assessment method ranged between 0.72 and 0.86 consistently over the years with no gender bias across science disciplines.

Table 1. Details of the modules and implementations

Module Title	Visualizations (N)	Investigations (N)	Prompts (N) Multiple-Choice	Open-Ended	Screenshot-Based	Implemented Week During the Pilot Study
Quantum Basics (QB)	6	7	9	10	4	1st week
Quantum Tunneling (QT)	4	6	8	5	3	2nd week
Semiconductors (SC)	9	6	12	6	1	5th week

Table 2. The Knowledge Integration (KI) Scoring Method at work

Score	KI State	KI Description	KI Scoring Criteria[1]	Pretest (%)	Posttest (%)
0	No information	Blank answers; Off-task remarks.	Blank	16	13
1	No idea/link	Elicited scientifically non-normative ideas or links.	A or only Zs	32	0
2	Partial link	Elicited scientifically normative ideas that were not connected.	One of the ideas from B, C, and D	32	40
3	Full link	Elaborated a link between two scientifically normative ideas.	Two of the ideas from B, C, and D	21	47
4	Complex link	Elaborated two or more links between three or more scientifically normative ideas.	All the ideas from B, C, and D	0	0

[1] Explanation ideas:
 A: Restatement (electrons go up and holes go down).
 B: Holes have positive charges.
 C: Holes (positive charges) are repelled by positive charges and attracted by negative charges.
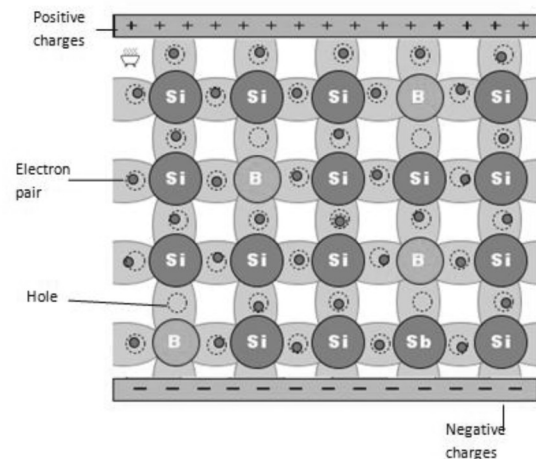 D: Holes move in the same direction as the applied field.
 Z: Alternative ideas.
  Holes move towards the positive.
  Holes want to become neutral again.
  Holes move in the opposite direction of the field.

In which direction would the holes in the semiconductor below travel? Note that an electric field is applied in the vertical direction.

Up
Down
Left
Right

Explain your answer.

Fig. 10. An example of an item that probes into students' understanding about charge carriers in semiconductors. This simulation is based on the classical molecular dynamics that treats electrons as Newtonian particles. Holes are modeled as potential wells that trap electrons. The open-ended part was scored from 0 to 4 based on the Knowledge Integration Scoring Method formulated in Table 2.

A test score was created as a sum of all scores a student received on the test. Reliability of the identical pre/post tests used in this pilot study was a Cronbach alpha value of 0.55 based on responses of 19 students. Reliability of the KI items used in this study was lower than that of the KI items used in the large scale testing mainly due to the small sample size involved in the pilot study rather than the quality of items given in the prior research on the KI assessment method [45, 51]. Reliability of a test mainly relates to estimated effect sizes being less well defined. The use of identical pre/post tests to report student learning gains has both positive and negative impacts on the study. On the positive side, researchers can take into account students' preexisting understanding of the science content being tested. On the negative side, students might improve their understanding by just taking the same test twice, which is called the 'test' effect. However, the test effect was not a concern in this study because nanotechnology is quite a difficult science subject to learn even with organized science courses [52–55]. After giving the same problems to college students in the mid-term and final exams on quantum mechanics concepts, Mason and Singh [56] discovered that 'most advanced students do not automatically use their mistakes as an opportunity for learning, repairing, extending, and organizing their knowledge structure (p. 760)'. Students in this study were not given solutions after the pretest. In addition, the KI assessment put more weight towards students' elaboration of their ideas in

explanations than choosing a correct answer, which is less prone to test score increase due to memorization [45, 57, 58].

The same scoring method was used for students' answers to all multiple-choice and open-ended prompts in the three MW modules. For the screenshot-based prompts that asked students to take and annotate a snapshot image from a visual simulation as an answer, a dichotomous scoring method was used. A total module score was a sum of all scores a student received within a module. Hence, each student had scores on the variables that represented his/her overall performance on the pretest (max = 60), the posttest (max = 60), the QB module (max = 53), the QT module (max = 32), and the SC module (max = 37).

Repeated measures *t*-tests were applied to the pretest and the posttest score variables. There was a significant improvement from pre- to posttests as measured on multiple-choice items (Effect Size = 1.02 Standard Deviation, p < 0.05), explanation items (Effect Size = 1.09 Standard Deviation, p < 0.01), and combined (Effect Size = 1.29 Standard Deviation, p < 0.01), as shown in Fig. 11. This indicates that students in this course significantly improved their understanding of quantum mechanics and semiconductor physics before and after the intervention using three MW modules as homework.

In order to isolate the effects of the modules, a variable was created to represent students' performance differences between pre- and posttests (the DIFFERENCE variable = posttest score—pretest score). Another variable was created to represent how well students performed during the entire course (the GRADE variable). The GRADE variable was based on the A, B, C, and D grades that the instructor gave at the end of the course based on student performance on mid-term, final, and homework. An analysis of covariance (ANCOVA) was performed on the DIFFERENCE vari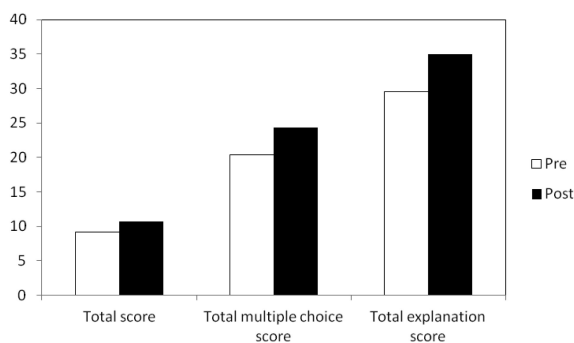able while the three module variables were entered as covariates that represent the fidelity of implementation and the GRADE variable as an independent variable. This analysis model explained 70% of the variations inherent in the DIFFERENCE variable.

Results show that a significant QB module effect, $F(5, 7) = 7.89$, $p < 0.05$, and a significant QT module effect, $F(5, 7) = 8.22$, $p < 0.05$, on the DIFFERENCE variable. These results mean that, after controlling for the GRADE effect, students who did better in the QB and QT modules gained significantly more between pre- and posttests than those who did not. No significant GRADE effect was found, $F(5, 7) = 2.79$, $p = 0.13$. The DIFFERENCE variable did not depend on the grades students received, meaning that students, on average, gained from pretest to posttest, regardless of how well they learned during the course. No significant SC module effect was found, $F(5,7) = 1.30$, $p = 0.29$. However, the effect of the SC module was not pronounced on the DIFFERENCE variable after controlling for students' course grades because of the content overlap between the course material and the SC module. Students significantly gained their understanding of concepts in the solid state physics but it was difficult to statistically differentiate between the understanding from the course material and the understanding from the SC module. In comparison, the students who benefitted from the QB and QT modules mostly improved their understanding of fundamental quantum phenomena on their own.

These results indicate that simulation-based experimentation can be successfully used for undergraduate students to develop integrated understanding of very difficult concepts in nanotechnology at their own pace without the involvement of heavy mathematics. In particular, the study shows a potential for supporting students who initially had a difficult time to form a mental representation of quantum phenomena. For example, a student mentioned the modules' contribution to the development of his understanding by saying that 'I liked that the modules not only provided visualizations of certain topics but allowed interactions with the user as well. I thought this was helpful in forming mental images of concepts.'

6. Conclusions

Formalism used to be the only way to teach concepts and visions in nanotechnology. Formalism, however, poses a learning barrier to many students who are not comfortable with heavy use of mathematical and theoretical analyses. This paper proposes a visual approach to teaching nanotechnology that may be widely applicable in K-16 education. Through interactive graphics generated by compu-

Fig. 11. Pre/posttest scores show learning gains through the MW modules.

ter simulation of nanoscale phenomena, this approach has the potential to allow more students, be they precollege students, non-science majors, or technician students, to learn about the fundamental concepts and farsighted ideas in nanotechnology without being bogged down in the difficulty of technical details. Preliminary results from a small-scale pilot study at the college level demonstrated the promising power of this approach. In particular, the results indicate that college students gained deeper understanding of abstruse quantum ideas from our visual quantum simulations.

Based on this pilot study, a follow-up quasi-experimental study that directly compares the effects of formal treatments and the visual approach is currently underway. Future research will use experimental designs with control groups to establish learning benefits of scientific visualizations approach [59] and design-based methods [60] to further improve the effectiveness of the simulations used in this study. In addition, the modules should be tested across student demographics and college settings to ensure that the learning benefits reported in this paper can be generalized to a greater student population.

References

1. E. Drexler, *Engines of Creation 2.0: The Coming Era of Nanotechnology*: WOWIO Books, 2007.
2. Battelle Memorial Institute and Foresight Nanotech Institute, http://www.foresight.org/roadmaps/, Accessed 26 April, 2012
3. E. Drexler, http://www.nanowerk.com/spotlight/spotid=15067.php, Accessed 26 April, 2012
4. E. Drexler, *Nanosystems: Molecular Machinery, Manufacturing, and Computation*, 1st ed.: Wiley, 1992.
5. C. Xie, R. F. Tinker, B. Tinker, A. Pallant, D. Damelin and B. Berenfeld, Computational Experiments for Science Education, *Science*, 332, 2011, pp. 1516–1517.
6. A. R. Leach, *Molecular Modeling: Principles and Applications*, 2nd ed.: Pearson Education, 2001.
7. E. Shipley and T. Moher, Instructional Framing for Nanoscale Self-Assembly Design in Middle School: A Pilot Study, in *Annual Meeting of the American Educational Research Association, March 24–28, 2008,* New York City, 2008.
8. R. P. Feynman, There's Plenty of Room at the Bottom, *Journal of Microelectromechanical Systems,* 1, 1992, pp. 60–66.
9. R. P. Feynman, R. D. Leighton and M. Sands, *The Feynman lectures on physics*, Addison-Wesley, Menlo Park, 1963.
10. D. C. Rappaport, *The Art of Molecular Dynamics Simulation*, Cambridge University Press, Cambridge, UK, 1997.
11. A. Arkhipov, P. L. Freddolino, K. Imada, K. Namba and K. Schulten, Coarse-Grained Molecular Dynamics Simulations of a Rotating Bacterial Flagellum, *Biophysical Journal,* 91, 2006, pp. 4589–4597.
12. A. Arkhipov, Y. Yin and K. Schulten, Four-Scale Description of Membrane Sculpting by BAR Domains, *Biophysical Journal,* 95, 2008, pp. 2806–2821.
13. J. G. Gay and B. J. Berne, Modification of the overlap potential to mimic a linear site-site potential, *Journal of Chemical Physics,* 74, 1981, pp. 3316–3319.
14. D. J. Cleaver, C. M. Care, M. P. Allen and M. P. Neal, Extension and generalization of the Gay-Berne potential, *Physical Review E,* 54, 1996, pp. 559–567.
15. C. Xie, http://www.concord.org/~qxie/papers/beyondlj.pdf, Accessed 26 April, 2012
16. A. Nealen, M. Müller, R. Keiser, E. Boxerman and M. Carlson, Physically Based Deformable Models in Computer Graphics, in *EUROGRAPHICS* Dublin, Ireland, 2005.
17. IBM, http://www.almaden.ibm.com/almaden/media/mirage.html, Accessed 26 April, 2012
18. N. Watanabe and M. Tsukada, Fast and stable method for simulating quantum electron dynamics, *Physical Review E,* 62, 2000, pp. 2914–2923.
19. L. Lehtovaara, J. Toivanen, and J. Eloranta, Solution of time-independent Schrödinger equation by the imaginary time propagation method, *Journal of Computational Physics,* 221, 2007, pp. 148–157.
20. Scanning Tunneling Microscopy, http://mw2.concord.org/tmp.jnlp?address=http://mw2.concord.org/public/part1/stm/index.cml (Java is required to open this module), Accessed 26 April, 2012
21. Molecular Self-Assembly, http://mw2.concord.org/tmp.jnlp?address=http://mw2.concord.org/public/part1/selfassembly/index.cml (Java is required to open this module), Accessed 26 April, 2012
22. Atomic Layer Deposition: A Virtual Experiment, http://mw2.concord.org/tmp.jnlp?address=http://mw2.concord.org/public/student/nano/alcvd.cml (Java is required to open this module), Accessed 26 April, 2012
23. J. L. Kolodner, Facilitating the Learning of Design Practices: Lessons Learned from an Inquiry into Science Education, *Journal of Industrial Teacher Education,* 39, 2002.
24. Algoryx Simulation AB, http://www.algodoo.com/wiki/Education, Accessed 26 April, 2012
25. J. Casperson and M. C. Linn, Using visualizations to teach electrostatics, *American Journal of Physics,* 74, 2006, pp. 316–323.
26. T. J. José and V. M. Williamson, Molecular visualization in science education: An evaluation of the NSF-sponsored workshop, *Journal of Chemical Education,* 82, 2005, pp. 937–942.
27. J. K. Gilbert, *Visualization in Science Education*: Springer, 2005.
28. C. E. Wieman, W. K. Adams and K. K. Perkins, PhET: Simulations That Enhance Learning, *Science,* 322, 2008, pp. 682–683.
29. C. E. Wieman and K. K. Perkns, A powerful tool for teaching science, *Nature Physics,* 2, 2006, pp. 290–292.
30. R. K. Lowe, Interrogation of a dynamic visualisation during learning, *Learning and Instruction,* 14, 2004, pp. 257–274.
31. M. C. Linn, H.-Y. Chang, J. Chiu, H. Zhang and K. McElhaney, Can Desirable Difficulties Overcome Deceptive Clarity in Scientific Visualizations?, in *Successful Remembering and Successful Forgetting: A Festschrift in Honor of Robert A. Bjork*, The Taylor & Francis Group, London, England, 2010.
32. M. Alavi and D. Dufner, Technology-mediated collaborative learning: A research perspective, in *Learning together online: Research on asynchronous learning networks.*, S. R. Hiltz and R. Goldman, Eds. Lawrence Earlbaum Associates, Mahwah, NJ, 2005.
33. R. Kozma, Students collaborating with computer models and physical experiments, in *Proceedings of the Conference on Computer-Supported Collaborative Learning 1999*, J. Roschelle and C. Hoadley, Eds. Erlbaum, Mahwah, NJ, 2000, pp. 314–322.
34. J. J. Williams and T. Lombrozo, The Role of Explanation in Discovery and Generalization: Evidence From Category Learning, *Cognitive Science: A Multidisciplinary Journal,* 34, 2010, pp. 776–806.

35. R. E. Mayer, Should There Be a Three-Strikes Rule Against Pure Discovery Learning? The Case for Guided Methods of Instruction, *American Psychologist*, **59**, 2004, pp. 14–19.

36. S. Papert, 'Situating Constructionism,' in *Constructionism*, I. Harel and S. Papert, Eds. Ablex Publishing Corporation, Norwood, NJ, 1991.

37. C. Xie and A. Pallant, Constructive Chemistry: A Case Study of Gas Laws, *@Concord*, **13**, 2009, pp. 12–13.

38. A. Greenberg, Integrating nanoscience into the classroom: perspectives on nanoscience education projects, *ACS Nano*, **3**, 2009, pp. 762–769.

39. Quantum Basics, http://mw2.concord.org/tmp.jnlp?address=http://mw2.concord.org/public/part1/etquantum/index.cml (Java is required to open this module), Accessed 26 April, 2012.

40. Quantum Tunneling, http://mw2.concord.org/tmp.jnlp?address=http://mw2.concord.org/public/part1/tunneling/index.cml (Java is required to open this module), Accessed 26 April, 2012.

41. Semiconductors, http://mw2.concord.org/tmp.jnlp?address=http://mw2.concord.org/public/part1/semiconductor/index.cml (Java is required to open this module), Accessed 26 April, 2012.

42. L. Dusenbury, R. Brannigan, M. Falco and W. B. Hansen, A review of research on fidelity of implementation: Implications for drug abuse prevention in school settings, *Health Education Research*, **18**, 2003, pp. 237–256.

43. C. L. O'Donnell, Defining, conceptualizing, and measuring fidelity of implementation and its relationship to outcomes in K-12 curriculum intervention research, *Review of Educational Research*, **78**, 2008, pp. 33–84.

44. W. T. Summerfelt, Program strength and fidelity to evaluation, *Applied Developmental Science*, **7**, 2003, pp. 55–61.

45. H.-S. Lee, O. L. Liu and M. C. Linn, Validating measurement of knowledge integration in science using multiple-choice and explanation items, *Applied Measurement in Education*, **24**, 2011, pp. 115–136.

46. L. O. Liu, H. S. Lee, C. Hofstetter and M. C. Linn, Assessing knowledge integration in science: Construct, measures, and evidence, *Educational Assessment*, **13**, 2008, pp. 1–23.

47. M. Linn, H.-S. Lee, R. Tinker, R. Husic and J. Chiu, Teaching and assessing knowledge integration in science, *Science*, **313**, 2006, pp. 1049–1050.

48. M. Linn, The Knowledge Integration Perspective on Learning and Instruction, in *The Cambridge Handbook of the Learning Sciences*, R. K. Sawyer, Ed. Cambridge University Press, New York, 2006, pp. 243–264.

49. H.-S. Lee, M. C. Linn, K. Varma and O. L. Liu, How does technology-enhanced inquiry instruction with visualizations impact classroom learning?, *Journal of Research in Science Teaching*, **47**, 2010, pp. 71–90.

50. O. L. Liu, H.-S. Lee and M. C. Linn, Multi-faceted assessment of inquiry-based science learning, *Educational Assessment*, **15**, 2010, pp. 69–96.

51. O. L. Liu, H.-S. Lee and M. C. Linn, Measuring knowledge integration: Validation of four-year assessments, *Journal of Research in Science Teaching*, **48**, 2011, pp. 1079–1107.

52. L. Deslauriers and C. E. Wieman, Learning and retention of quantum concepts with different teaching methods, *Physical Review Special Topics—Physics Education Research*, **7**, 2011, p. 010101.

53. [53]M. Ayene, J. Kriek, and B. Damtie, Wave-particle duality and uncertainty principle: Phenomenotraphic categories of description of tertiary physics students' depictions, *Physical Review Special Topics—Physics Education Research*, **7**, 2011, p. 020113.

54. S. B. McKagan, K. K. Perkins and C. E. Wieman, Design and validation of the quantum mechanics conceptual survey, *Physical Review Special Topics—Physics Education Research*, **6**, 2010, p. 020121.

55. C. Baily and N. D. Finkelstein, Teaching and understanding of quantum interpretations in modern physics courses, *Physical Review Special Topics—Physics Education Research*, **6**, 2010, p. 010101.

56. A. Mason and C. Singh, Do advanced physics students learn from their mistakes without explicit intervention?, *American Journal of Physics*, **78**, 2010, pp. 760–767.

57. S. Embretson and J. Gordin, Improving construct validity with cognitive psychology principles, *Journal of Educational Measurement*, **38**, 2001, pp. 343–368.

58. M. C. Rodriguez, Construct equivalence of multiple-choice and constructed-response items: A random effects synthesis of correlations, *Journal of Educational Measurement*, **40**, 2003, pp. 163–184.

59. T. D. Cook and D. T. Campbell, *Quasi-Experimentation: Design & analysis issues for field settings*. Houghton Mifflin, Boston, MA, 1979.

60. A. Collins, D. Joseph and K. Bierlaczyc, Design research: Theoretical and methodological issues, *Journal of the Learning Sciences*, **13**, 2004, pp. 43–76.

Charles Xie is Senior Scientist at the Concord Consortium. He holds a Ph.D. in materials science from the University of Science and Technology, Beijing. His work involves research and development of effective educational technology based on computational science, computer-aided design and fabrication, scientific imaging, augmented reality, and natural user interfaces. He is the Principal Investigator of the NSF project that funded this work (grant number DUE-0802532), as well as the creator of the Molecular Workbench software.

Hee-Sun Lee is Visiting Assistant Professor in the Physics Department at the University of California, Santa Cruz, and was Assistant Professor in the Education Department at Tufts University. She holds a Ph.D. in science education and an MS in Physics from the University of Michigan, Ann Arbor. Her research addresses design, implementation, assessment, and evaluation of innovative science curricula at secondary and higher education levels and design and validation of educational research instruments.