A VISUAL APPROACH TO NANOTECHNOLOGY EDUCATION

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Abstract: 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 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 recommended. Preliminary results from a pilot study at the college level demonstrated the promising power of this approach.

INTRODUCTION

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

A solid foundation is critically important to students. They 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 vision 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 this exciting vision.

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 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 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 form most students can learn from.

This work is based on the *Molecular Workbench* (MW) software (http://mw.concord.org) [5], which 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. Different 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.

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.

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. The simulations of fullerenes such as carbon nanotubes (Figure 1) and buckyballs generally require this model.

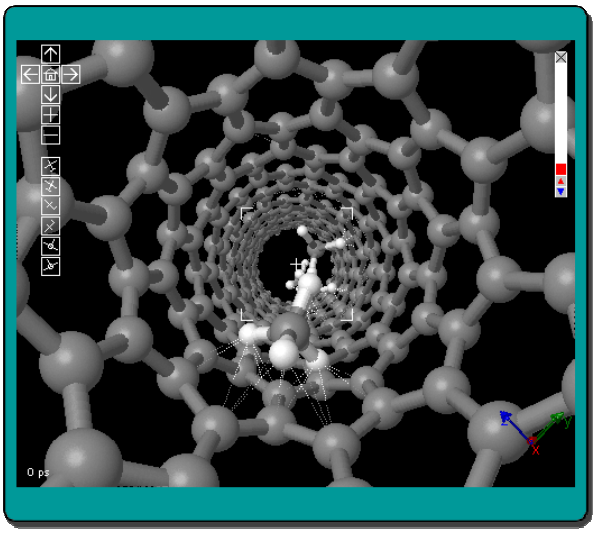


Figure 1. An all-atom molecular dynamics simulation of motion of methane molecules in a carbon nanotube.

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 supercomputing to come to schools. First, with Moore's Law approaching the limit, traditional desktop computers in schools are not expected to get faster any time soon. Second, more schools are using tablets that are actually powered by downgraded 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 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.

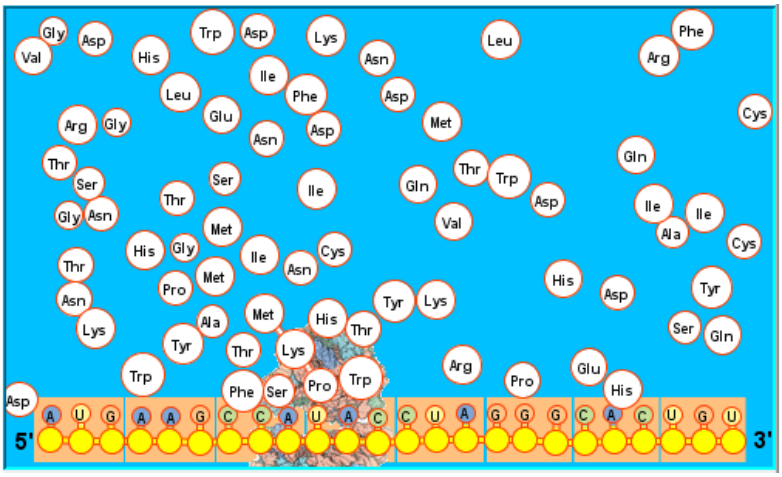


Figure 2. A coarse-grained dynamics simulation of translation (making proteins from messenger RNA). Each amino acid, RNA base, and RNA backbone are represented by a particle. The amino acids randomly bounce into the ribosome site and the one that matches the current RNA triplet will be attached to the growing polypeptide. The solvent is not explicitly modeled.

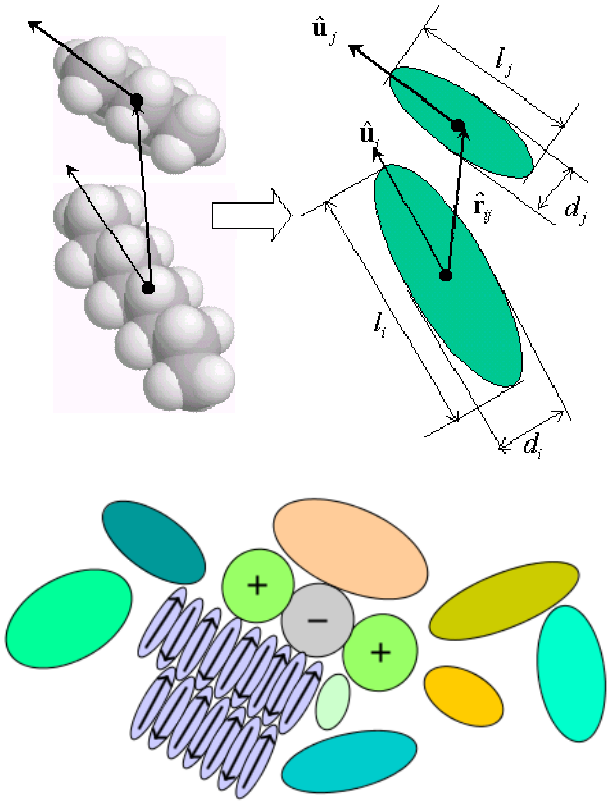


Figure 3. The Gay-Berne potential provides another coarse-grained model. The "+/-" signs represent charges, whereas the arrows electrical dipole moments.

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 Figure 3). The potential has been widely used to 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 Figure 3).

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 explore.

Most macromolecules are soft—they vibrate, react, deform, fold, and assemble. In many cases, only the molecular surfaces are important in affecting the intermolecular interactions and dynamics. There is rarely a need for students to know the details of the atoms inside the bulk that mostly provide the mass and structural support.

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 Figure 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, and so on.

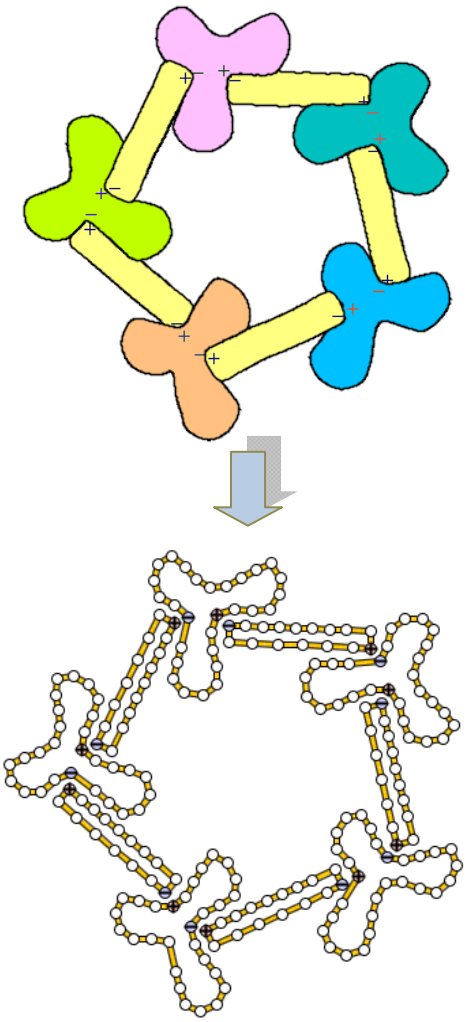


Figure 4.The mass-spring model is used to discretize 2D soft bodies (the angular constraints are not shown). Given physical properties, the self-assembly of these soft bodies can be simulated.

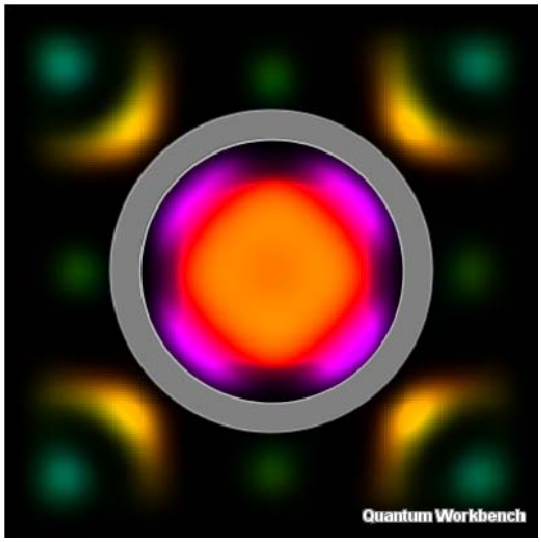


Figure 5. Quantum dynamics supplements molecular dynamics to provide visualizations for quantum concepts. The image shows a snapshot of the quantum wave in a curricular container with a finite barrier height. The wave is colored by its phase.

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 nanotechnology 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]. Figure 5 shows a 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.

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 our approach demonstrates its unique power.

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 microscopes for 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 (Figure 6). This simulation uses the Imaginary Time Propagation me-

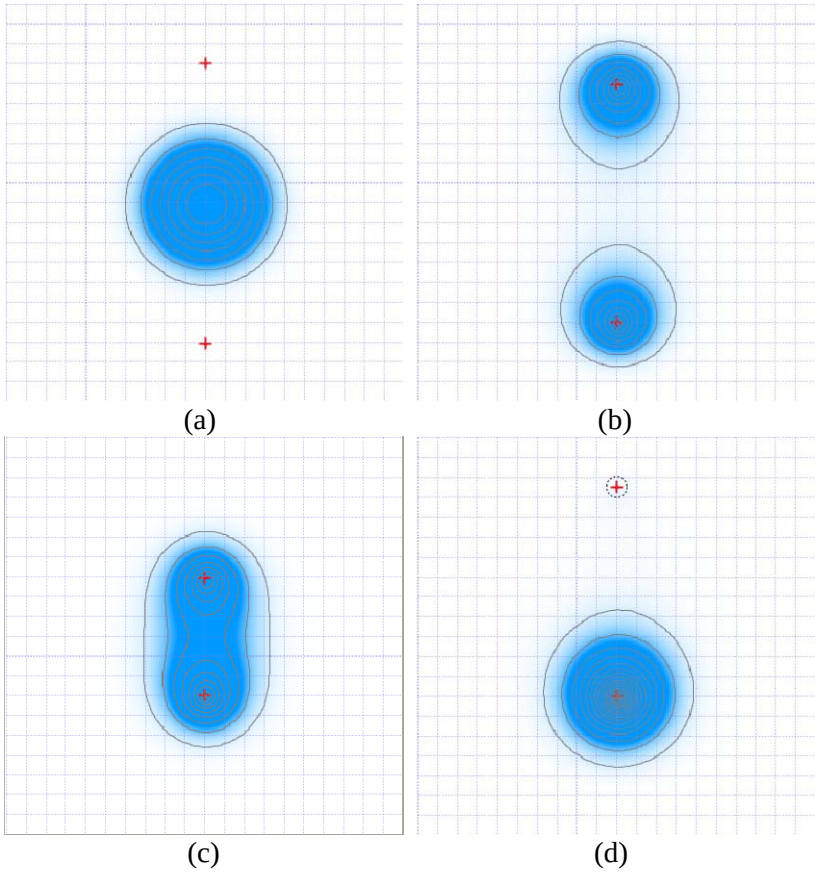


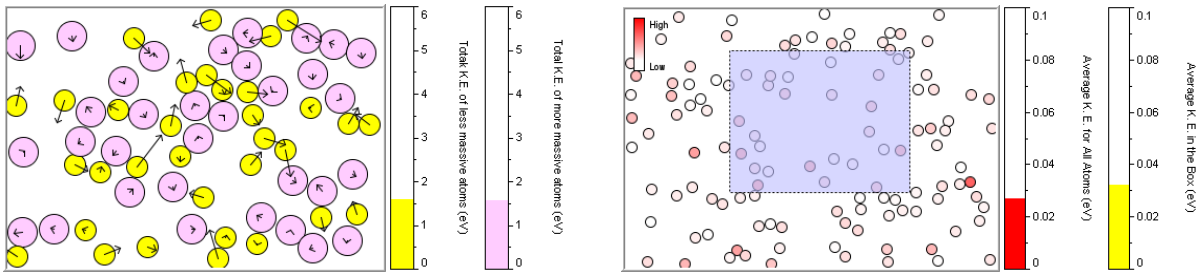
Figure 6. This interactive simulation allows students to discover possible states of a 2D quantum system. Because the quantum mechanics calculation is done in real time, the shape of the electron cloud (represented by the blue haze) dynamically responds to the user's drag-and-drop of the protons (represented 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.

thod 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.

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.



(a) (b)

Figure 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.

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. Figure 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 (Figure 7a). The second illustrates that the average kinetic energy is the same everywhere for any subset of particles in a container that has reached thermal equilibrium (Figure 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 in Figure 7. Making sense of these simulations somehow resembles the learning experience with TinkerPlots [20], except that the data produced by molecular dynamics have built-in physical meanings.

Nanoelectronics

Nanoelectronics is an important branch of nanotechnology that holds the promise of making even more powerful computers in the future. The study of 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 molecular dynamics or the quantum dynamics method available in MW. The molecular dynamics simulation shows the classical particle view of electron flow, whereas the quantum dynamics simulation presents a novel wave view of quantum transport. Acute readers may notice that in the quantum simulation there may be a weak tunneling current even if the transistor is in the off state.

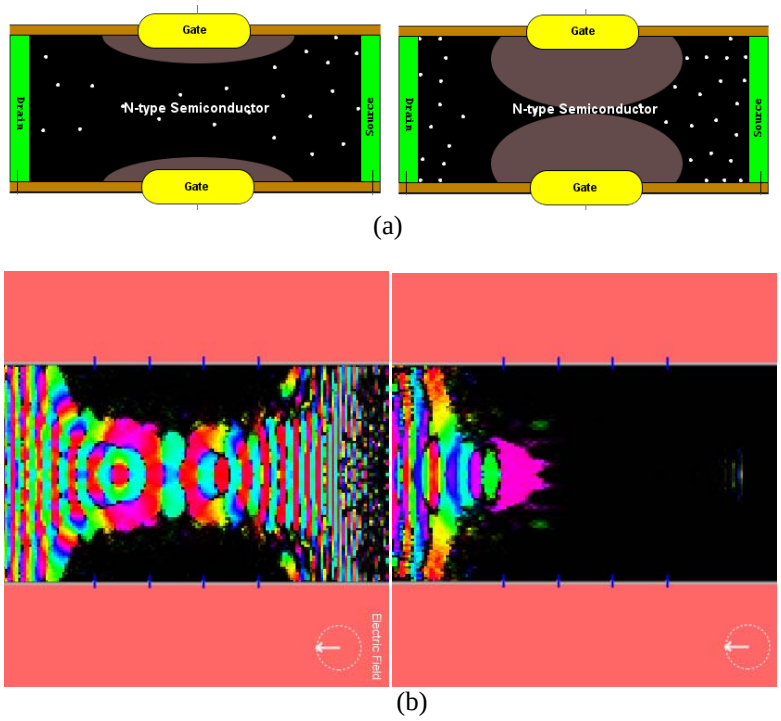


Figure 8. (a) A classical molecular dynamics simulation of a JFET. The small white dots represent electrons. (b) A quantum dynamics simulation of a JFET. The electron wave is colored by its phase. In both simulations, students can adjust the gate voltage to switch the transistor on (the left images)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

Virtual nanotechnology experiments and nanosystem designs

We have developed simulations for teaching scanning tunneling microscopy [21], electrostatic self-assembly [22], and atomic layer deposition [23]. These simulations can supplement lecture or laboratory to provide additional opportunities of learning. The interactivity design of some of these virtual experiments even simulates laboratory procedures. Hence, they may be useful to technician training as well.

As pointed out in the Introduction, nanotechnology education should not just teach fundamentals. Perhaps more importantly, it should also pass the exciting vision of nanotechnology to students. Futuristic nanosystems, such as those conceptual nanomachines conceived in Drexler's foundational book [4], can be

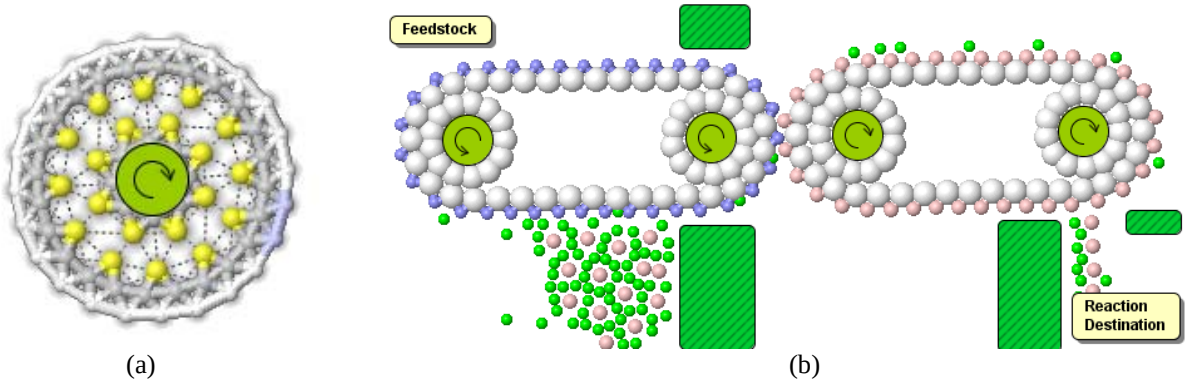


Figure 9. (a) An internal nanogear that resembles Figure 1.1 in Drexler's defining book about nanosystems. The dashed lines show the van der Waals interactions that facilitate the "transmission" mechanism. (b) Two nano conveyor belts that actively sort and transport a certain type of feedstock molecules,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

brought to the classroom through simulations to provide inspirations. We have created a collection of fictitious nanomachines such as nanogears and nano conveyor belts (Figure 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 [24]. 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 [25].

INSTRUCTIONAL STRATEGIES USING SIMULATIONS

Visual simulations are often attractive presentations to teachers and students. However, the attraction in the first impression is not a guarantee of learning. 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, can play a positive role on amplifying the power of visual simulations.

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

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 using the simulation:

1) "Students as passengers in a taxi cab": The teacher shows students a simulation and tells 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 interactive opportunities provided by the simulation. In many cases, this mediation can be used to make a "screenplay" that scaffolds effective lecture.

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 is usually more effective than open inquiry [26]. Guided inquiry

uses clear goals, careful scaffolding, ongoing assessment, and teacher intervention to lead students to independent learning. 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 pairs 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. 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.

RESULTS FROM A PILOT STUDY

Although the ideas of nanotechnology have been infused into many existing courses in science and engineering [27], 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 of the difficulties in obtaining sufficient funding to recruit and train enough number of teachers and students across grade levels.

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 physics, 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 decided to use three online MW modules as homework for individual students to gain more robust understanding of fundamental quantum concepts as they related to semiconductor devices. The three MW modules were Quantum Basics (QB), Quantum Tunneling (QT), and Semiconductors (SM). The QB module covers probability waves, diffraction and interference, tunneling, bound states, and excited states [28]. The QT module covers factors that affect tunneling, tunneling leakage in computer chips, tunnel injection and release, and nanopore DNA sequencing [29]. The SM module covers thermal excitation, intrinsic and doped semiconductors, electron holes, P-N junctions, and the energy band theory [30]. The instructional design of the three modules followed 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 causality. 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.

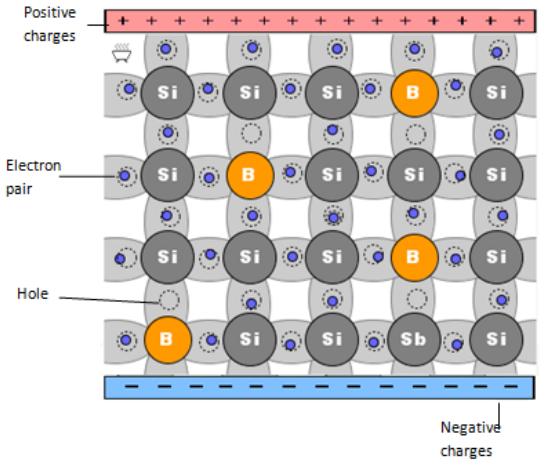
Table 1. Details of the modules and implementations.

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

In order to investigate the impact of these modules on student learning, we administered an identical paper-and-pencil test in the first and the last class of the course. 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 behaviors) and solid state physics (e.g., metals, semiconductors, transistors, and P-N junctions). To consider student engagement with the MW modules, we collected student answers to all of the prompts embedded in them. 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 SM 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 [31, 32]. The method is based on the Knowledge Integration Theory [33, 34] 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 [35]. 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 Figure 10). The higher the KI score, the more integrated the student's understanding.

A test score was created as a sum of all scores a student received on the test. 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 SM module (max = 37).



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

(1) Up
(2) Down
(3) Left
(4) Right

Explain your answer.

Figure 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.

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

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, $p < .05$), explanation items (Effect Size = 1.09 Standard Deviation, $p < .01$), and combined (Effect Size = 1.29 Standard Deviation, $p < .01$), as shown in Figure 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.

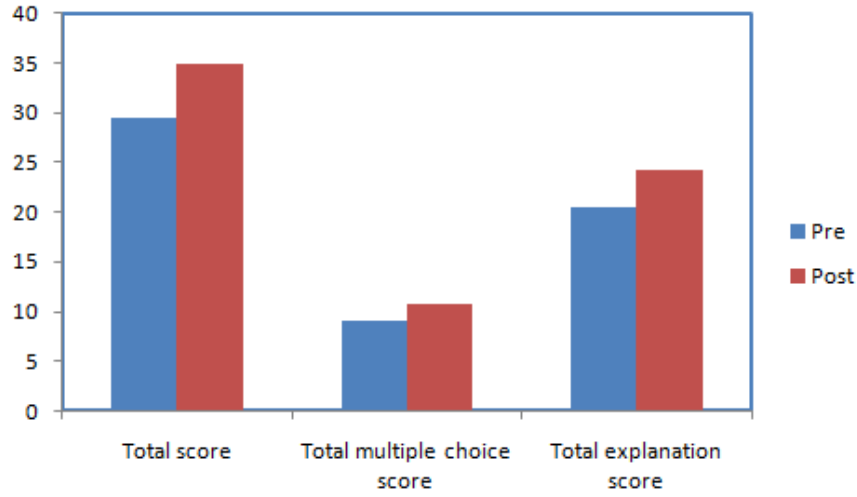


Figure 11. Pre/posttest scores showed learning gains.

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 variable while the three module variables were entered as covariates 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, $F(5,7) = 7.89$, $p < .05$, and a significant QT module effect, $F(5,7) = 8.22$, $p < .05$, 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, $F(5,7) = 2.79$, $p = .13$. The DIFFERENCE variable did not depend on the grades students received, meaning that students, on average, gained from pretest to posttest, regardless of their course grades. No significant SM module effect was found, $F(5,7) = 1.30$, $p = .29$, however. The effect was not pronounced on the DIFFERENCE variable after controlling for students' course grades because of the content overlap between the course material and the SM 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 SM module. In comparison, the students who benefitted from the QB and QT modules mostly improved their understanding of fundamental quantum phenomena on their own.

SUMMARY

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 computer 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 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.

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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, "Productive Nanosystems: A Technology Roadmap," 2007.

[3] E. Drexler, "How to Study for a Career in Nanotechnology," in *Metamodern: The Trajectory of Technology*, Nanowerk, 2010. (http://www.nanowerk.com/spotlight/spotid=15067.php)

[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,* vol. 332, pp. 1516-1517, 2011.

[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,* vol. 1, pp. 60-66, 1992.

[9] R. P. Feynman, R. D. Leighton, and M. Sands, *The Feynman lectures on physics*. Menlo Park: Addison-Wesley, 1963.

[10] D. C. Rappaport, *The Art of Molecular Dynamics Simulation*. Cambridge, UK: Cambridge University Press, 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,* vol. 91, pp. 4589-4597, 2006.

[12] A. Arkhipov, Y. Yin, and K. Schulten, "Four-Scale Description of Membrane Sculpting by BAR Domains," *Biophysical Journal,* vol. 95, pp. 2806-2821, 2008.

[13] J. G. Gay and B. J. Berne, "Modification of the overlap potential to mimic a linear site-site potential," *Journal of Chemical Physics,* vol. 74, pp. 3316-3319, 1981.

[14] D. J. Cleaver, C. M. Care, M. P. Allen, and M. P. Neal, "Extension and generalization of the Gay-Berne potential," *Physical Review,* vol. E54, pp. 559-567, 1996.

[15] C. Xie, "Molecular Dynamics Simulations Beyond the LennardJones Particles," unpublished manuscript: http://www.concord.org/~qxie/papers/beyondlj.pdf

[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, "IBM Scientists Discover Nanotech Communication Method." http://www.almaden.ibm.com/almaden/media/mirage.html

[18] N. Watanabe and M. Tsukada, "Fast and stable method for simulating quantum electron dynamics," *Physical Review E*, vol. 62, pp. 2914–2923, 2000.

[19] L. Lehtovaara, J. Toivanen, and J. Eloranta, "Solution of time-independent Schrödinger equation by the imaginary time propagation method," *Journal of Computational Physics*, vol. 221, pp. 148-157, 2007.

[20] TinkerPlots, "TinkerPlots® Dynamic Data Exploration," Key Curriculum Press, 2011 (http://www.keypress.com/x5715.xml)

[21] C. Xie, "Scanning Tunneling Microscopy," 2010 http://mw2.concord.org/tmp.jnlp?address=http://mw2.concord.org/public/part1/stm/index.cml

[22] E. Rosenbaum and C. Xie, "Molecular Self-Assembly," 2011, http://mw2.concord.org/tmp.jnlp?address=http://mw2.concord.org/public/part1/selfassembly/index.cml

[23] E. Rosenbaum and C. Xie, "Atomic Layer Deposition: A Virtual Experiment." 2006, http://mw2.concord.org/tmp.jnlp?address=http://mw2.concord.org/public/student/nano/alcvd.cml

[24] J. L. Kolodner, "Facilitating the Learning of Design Practices: Lessons Learned from an Inquiry into Science Education," *Journal of Industrial Teacher Education*, vol. 39, 2002.

[25] Algoryx Simulation AB, "Algodoo for Education: Activate Scientific Thinking with Quick and Easy Experimentation." 2011, http://www.algodoo.com/wiki/Education

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

[27] A. Greenberg, "Integrating nanoscience into the classroom: perspectives on nanoscience education projects," *ACS Nano*, vol. 3, pp. 762-769, 2009.

[28] C. Xie, "Quantum Basics." 2010, http://mw2.concord.org/tmp.jnlp?address=http://mw2.concord.org/public/part1/etquantum/index.cml

[29] C. Xie, "Quantum Tunneling." 2010, http://mw2.concord.org/tmp.jnlp?address=http://mw2.concord.org/public/part1/tunneling/index.cml

[30] C. Xie, "Semiconductors." 2010, http://mw2.concord.org/tmp.jnlp?address=http://mw2.concord.org/public/part1/semiconductor/index.cml

[31] 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*, vol. 24, pp. 115-136, 2011.

[32] L. O. Liu, H. S. Lee, C. Hofstetter, and M. C. Linn, "Assessing knowledge integration in science: Construct, measures, and evidence," *Educational Assessment,* vol. 13, pp. 1-23, 2008.

[33] M. Linn, H.-S. Lee, R. Tinker, R. Husic, and J. Chiu, "Teaching and assessing knowledge integration in science," *Science,* vol. 313, pp. 1049-1050, 25 August 2006.

[34] M. Linn, "The Knowledge Integration Perspective on Learning and Instruction," in *The Cambridge Handbook of the Learning Sciences*, R. K. Sawyer, Ed. New York: Cambridge University Press, 2006, pp. 243-264.

[35] 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,* vol. 47, pp. 71-90, 2010.