Computer-based Tools for Nanotechnology Education and Research

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***Abstract* - The interdisciplinary nature of nanotechnology presents a difficulty when developing a curriculum or performing research. The field of study requires an in-depth understanding of fundamental biology, chemistry, physics, and engineering to comprehend phenomena at the nano-scale. Furthermore, the difficult and sometimes exotic math principles behind the engineering and physics, in particular, can be a stumbling block. This article details new key visual and computational tools to overcome these obstacles. The computer-aided approach helps to visualize the nano-scale and gives flexibility in communication of material. Open-source resources such as NanoEngineer-1 and the Nanohub have been proven useful for both researchers and students alike. In addition, the computer-aided approach can be a good medium between the excessively broad and the complex and can introduce students to standard industrial tools, such as Matlab.**

Index Terms – nanotechnology education, visualization, computational tools, Matlab

INTRODUCTION

The defining characteristic of nanotechnology is extreme dimension. According to the National Nanotechnology Initiative (NNI), nanotechnology involves materials with dimensions ranging from 1 nanometer (nm) to approximately 100 nm [1]. A common misconception about nanotechnology is that dimension alone makes a material "nano." The properties of the material by virtue of its dimensions must be significantly different than bulk materials. In essence, nanotechnology involves the design and manipulation of atoms to perform specific functions or create materials with unique properties. At the macroscopic scale as well as the microscopic scale, the properties of materials are uniform and predictable. However, at the nano-scale or atomic level, materials exhibit novel properties. Applications of nanotechnology take advantage of these unique properties to create new materials or improve the functionality and efficiency of existing materials. From medicine and alternative energy to electronics and even textiles, nanotechnology has already shown great potential and proven its worth to society. Applications are supported by solid research and development processes, but research is built on a fundamental education core. In the field of nanotechnology, it is this core education which presents the first real difficulty, particularly in undergraduate studies. The major impediment to developing an education core is nanotechnology's interdisciplinary nature. The field is so rich in biology, chemistry, physics, and engineering that to obtain an in-depth understanding of the phenomena at the nano-scale, students would need as a prerequisite a healthy amount of all four fundamental disciplines. Furthermore, the difficult math principles behind the engineering and especially the physics can be a stumbling block for undergraduates. The following sections of this report detail a process as well as methods for infusing nanotechnology into undergraduate studies. The process should be gradual, and the methods should involve computer-aided visualization and hands-on lab experiences with industry standard computer tools and lab equipment.

First, it is important to realize that nanotechnology is a synergism of two sub-disciplines, nanoscience and nanoengineering, which share a common foundation. nanoscience refers to the discovery of nano-scale phenomena while nanoengineering involves the production and integration of nanomaterials into engineering systems for applications. Each discipline contains specialties mutually exclusive with the other discipline. Prior to pursuing one these disciplines, one should have as a perquisite all calculus classes as well as linear algebra, chemistry, general physics, and quantum physics. The greatest learning curve among all nanotechnology requirements is associated with quantum physics. Quantum physics by far plays the most important role in nanotechnology as material properties are no longer governed by traditional Newtonian dynamics. The pervading aspect of quantum physics in nanotechnology presents a difficulty to some chemists as well as many engineers and biologists entering the realm of nanotechnology. Though difficult, the physics of nanotechnology cannot be overlooked. It is an essential requirement for any work in any facet of nanotechnology.

Aside from the coursework requirements, a curriculum should emphasize two other elements without which could hinder both academic and career development – visualization of the nano-scale and experience with industry standard computational tools and lab equipment. The ability to visualize in one's mind the structure of a nanomaterial or the actions and results of various nano-scale phenomena is extremely important. Unlike other disciplines such as engineering and biology, there are a limited amount of hands-on exercises readily available to perform in the classroom for visual reinforcement of particular theories.

Additionally, the equipment necessary for the hands-on experiences in the lab exercises are not cheap. Many schools have limited or altogether nonexistent budgets for creating clean rooms or acquiring quality microscopy equipment for students to use. Nevertheless, a solid nanotechnology should include some semblance of experience with industry standard tools as well as give students every opportunity to acquire the skill of visualization. The next section examines particular methods for overcoming the difficulties presented by the quantum physics, shows techniques for promoting visualization, and suggests cost-effective tools for computational and hands-on lab experiences.

METHODS

Though Oakland University currently does not have a full-fledged nanotechnology program, it was apparent that an introductory level course could be effectively used to peak interest in students. The drawback of an introductory class, however, is that they occur within the first two or three years of undergraduate programs. With this in mind, students will not have all the prerequisites needed for an in-depth study. The most important requirement most students will lack is quantum mechanics. Although quantum mechanics is typically reserved for upper level undergraduate or graduate students, the principles and results of quantum mechanics can be effectively introduced through applicable images, animations, computer simulations, and other tools. Similar techniques are also important for the conceptualization of nano-scale materials and devices. The incorporation of these tools into classroom material as well as lab modules and supplemental interactive online material will prove to be crucial to a proper education.

Nanohub

One of the foremost resources in the world for nanotechnology is nanoHUB. NanoHUB is an NSF-funded online resource with animations and simulation tools for quantum mechanical concepts, nano-devices, and nano-electromechanical systems (NEMS) among other things [2]. The online infrastructure was created by the Network for Computational Nanotechnology (NCN), a collection of universities seeking to develop nanotechnology through innovative collaboration. In addition to world-class simulation tools, the site contains downloadable nanotechnology-related lectures with audio. The main benefit of nanoHUB lies in its internet platform which greatly eases integration into the classroom.

Jmol

Jmol is another web-based resource which allows users to interactively rotate 3D nanomaterials, molecules, and devices. The open-source Java applet only requires file inputs with the locations and types of atoms in the molecules. Typical input files include XYZ and PDB formats [3]. The Jmol applet will interpret the types of atoms in each file and attribute a color according to conventional standards (i.e. carbon is gray and hydrogen is white). Jmol is extremely simple to integrate into existing course websites, and the input files are small so as to not clutter server space. The documentation provided at the official Jmol website gives clear instructions which even the inexperienced web designer could understand.

NanoEngineer-1 (NE-1)

Because nanotechnology is interdisciplinary, software applications which bridge the gap between each discipline and still provide the ability to perform computational tasks will prove to be important for the future. NanoEngineer-1 (NE-1) produced by Nanorex is also an open-source program and contains an easy-to-learn CAD interface. NE-1 has the capability of modeling and simulating 3D nanocomposite structures, including DNA and other biological molecules [4]. NE-1 is a dual purpose tool as it will improve a student’s visualization ability while performing heavy computational operations. The software will serve as an excellent platform for many lab modules on select nanotechnology topics.

Matlab

Though widely used as strictly a modeling and simulation tool for various applications and industry, Matlab has a nice combination of high-level programming and 3D graphics capabilities that allows a user to create meaningful animations of physical phenomena based on quantum mechanical principles. One of the difficulties of simulating quantum mechanical systems is the amount of data associated with the number of dimensions. Matlab has excellent data handling capabilities as well as linear algebra and optimization functions to adequately solve quantum mechanical problems. It is a widely used tool in industry to perform computationally intensive tasks and deliver results quicker than programming in languages such as C, C++, and Fortran.

Microscopy

One of the most effective ways to promote visualization is to actually directly experiment with imaging various sample of material. Richard Feynman, in his famous address entitled “There’s Plenty of Room at the Bottom,” gave motivation for developing instruments which could image and manipulate at the nano-scale. In the 1980s, about thirty years after Feynman’s address, the first viable tools were developed. Today, scanning tunneling microscopy (STM) and atomic force microscopy (AFM) play an important role in education and research. STM operates by the quantum phenomenon of tunneling. When a very fine conducting tip is brought in close proximity to a surface, a tunneling current can occur. The magnitude of current is directly related to the distance between the tip and sample; therefore, by monitoring the measured current, one can find the topology of the surface. Unfortunately, since the STM is based on conduction, the sample must also be a conductor or semiconductor. The AFM, however, is much more versatile, allowing many types of materials. Similar to STM, the AFM contains a beam with a sharp tip which scans the surface of the sample. Atomic forces (i.e. van der Waals forces) cause the beam to deflect toward or away from the sample. The tiny deflections are amplified and detected through a laser system. Knowing the deflection as well as the rigidity of the beam (i.e. Young's modulus and characteristic spring constant), one can determine the original force through the well known Hooke's Law. The design of the microscopy instruments themselves present opportunities for education, but incorporating these imaging techniques early in one's education is invaluable.

RESULTS

While nanoHUB is an excellent tool in its own right and can be incorporated into any pertinent discussion, the other aforementioned tools have been integrated into a website geared specifically for an introductory nanotechnology class at Oakland University. Entitled NanOU, the site is authored by students, and it provides the necessary platform to disseminate in-depth information on select topics in nanotechnology and supplemental educational materials such as images, animations as well as descriptions of tangible applications and relevant nanotechnology news.

Educational Supplements

By far the most effective tools for developing visualizations of nanotechnology for the website have been Matlab and Jmol. A number of examples will demonstrate the fruitfulness of Matlab. Figure 4(a) and (b) shows the first and last images, respectively, of an animation developed in a Matlab example. As the width of an infinite 1D potential well decreases, the magnitude of the energy levels increase and become more discrete. This animation shows why energy levels in bulk materials are considered to be continuous. Figure 4 is important for demonstrating the application of quantum dots. A typical quantum dot is composed of CdSe (cadmium selenide), a compound semiconductor. Variations of the energy bandgap of bulk CdSe due to size are negligible. When stimulated by energy, bulk CdSe emits electromagnetic radiation at the same frequency. The bandgap of quantum dots, however, is tunable. Remove a few atoms to decrease its size, and the bandgap increases. The corresponding radiation emitted as a result of external stimuli is different than that of bulk CdSe. Figure 2 shows another visualization which is used to describe how the density of states in a material is found. The green spheres do not correspond to position here but rather to unique quantum states of a material. The density of states problem is a problem of finding the number of states in the interval of E and $E + dE$. In k-space, the interval is simply k and $k + dk$. In three dimensions, k represents the radius of a sphere in k-space and dk is the thickness of the sphere. Hence, a shell is created which encloses a certain amount of quantum states in an infinitesimal interval. Dividing the volume of the shell by the volume of a unit cell gives the density of states. The density of states is of prime importance for nanoelectronics in particular. The amount of current which can pass through the channel of a single transistor, for example, is directly related to the number of available states within the channel. The action of a nanotransistor can also be effectively portrayed through simulations. In an introductory level course, it is beneficial to consider the simplest nanotransistor possible, in which the channel only consists of one or two atoms. In this scenario the density of states can be counted on one hand, and the output of a transistor under varying conditions can be simulated. Figure 3 demonstrates results from the simulation

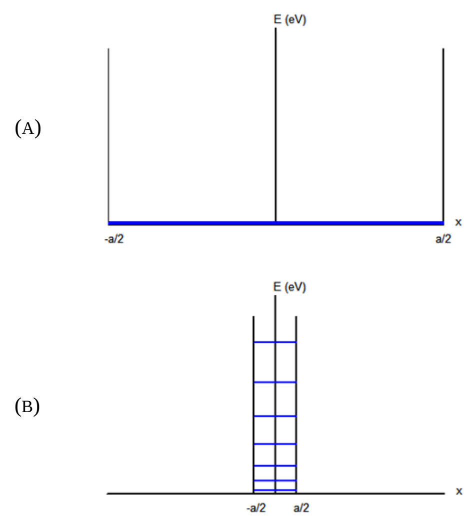


FIGURE 1
SNAPSHOTS TAKEN FROM AN ANIMATION DEPICTING (A) THE FIRST SEVEN ENERGY LEVELS OF AN INFINITE POTENTIAL WELL AND (B) THE SAME SEVEN LEVELS WHEN THE WELL WIDTH DECREASES [5]

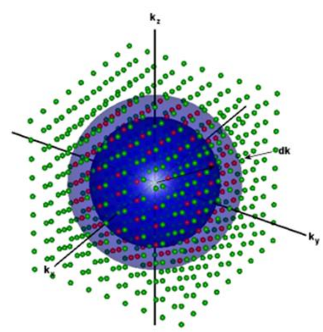
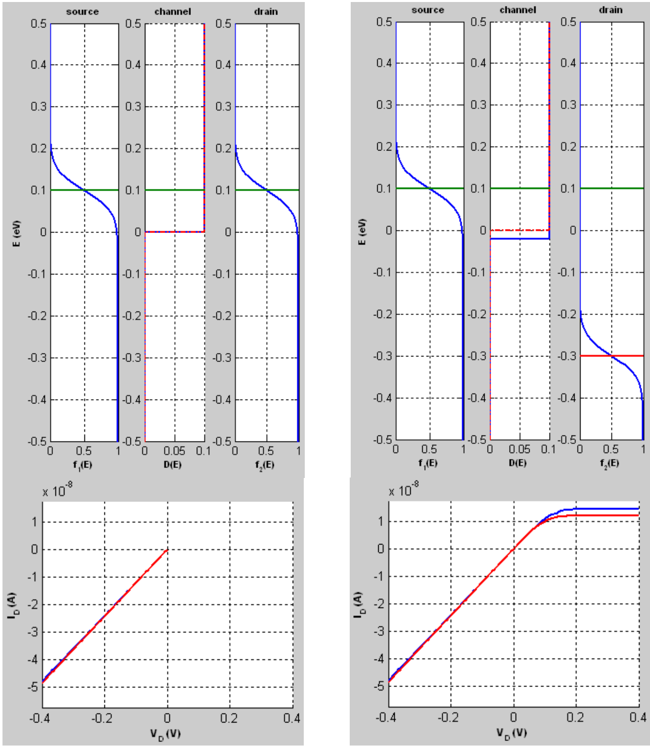


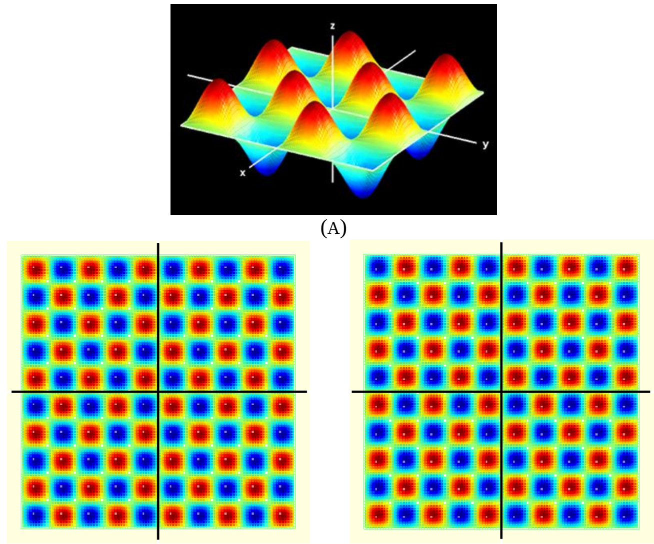
FIGURE 2
A REPRESENTATION OF THE TECHNIQUE FOR FINDING DENSITY OF STATES [6]



(A) (B)

FIGURE 3
SNAPSHOTS OF A TRANSISTOR ANIMATION OUTPUT WHEN (A) SOURCE AND DRAIN VOLTAGES ARE EQUAL AND (B) WHEN DRAIN VOLTAGE IS GREATER

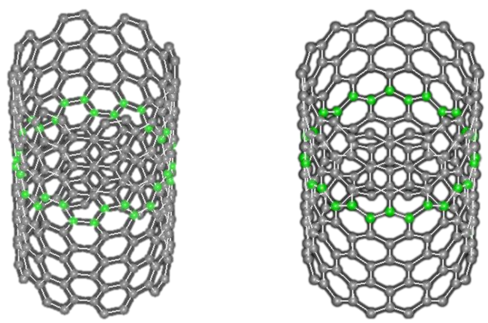
of a transistor using a simplified channel as voltages on the source and drain inputs are varied. In Figure 3(b), a larger number of available states increases the current level. Figure 4 shows a plot of the second energy level in a 2D potential well. Though the mathematical formalism of the potential well may not be fully covered in an introduction to nanotechnology, the results and bearing of the potential well on properties of materials should not be overlooked. Figure 4(b) displays time-dependent results of the 2D potential well animation. Not only is Matlab useful for portraying phenomena associated with nanoscience, but it is effective in creating depictions of structures of molecules and nanomaterials. Among of the most researched materials have been carbon nanotubes. Figure 5 displays two varieties of one of the earliest discovered nanomaterials – the carbon nanotube. Depending on the orientation of atoms along the axis of the nanotube, the nanotubes properties differ. Zigzag nanotubes tend to be metallic while most armchair nanotubes are semiconductors. Figure 6 gives another great Matlab example of a polymer with of a hydrophobic tail and hydrophilic head. Jmol is also an excellent tool to display various structures. Figure 7 gives an illustration of a Jmol product. The structure is a miniaturized version of a universal joint composed nearly entirely of carbon. The NanOU website has integrated a full-screen Jmol applet. By clicking on a structure, the user can interactively rotate the structures.



(A)

(B)

FIGURE 4
REPRESENTATIONS OF THE SOLUTIONS TO THE 2D POTENTIAL WELL PROBLEM. (A) DEPICTS A LOWER ENERGY SOLUTION WHILE (B) SHOWS SNAPSHOTS OF TIME DEPENDENT RESULTS OF A HIGHER ENERGY SOLUTION [7]



(A) (B)

FIGURE 5
REPRESENTATIONS OF AN (A) ARMCHAIR NANOTUBE AND (B) A ZIGZAG CARBON NANOTUBE [8]

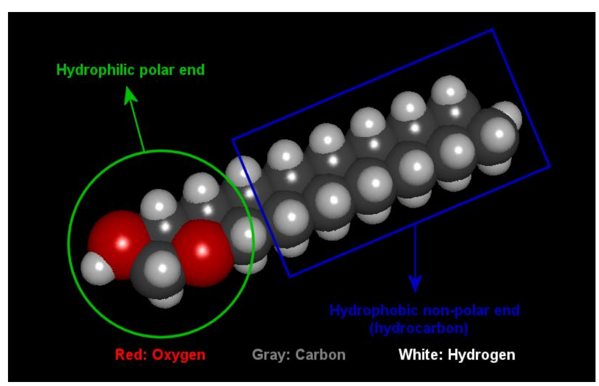


FIGURE 6
A POLYOXYETHYLENE MOLECULE DEMONSTRATING HYDROPHILIC AND HYDROPHOBIC STRUCTURE [9]

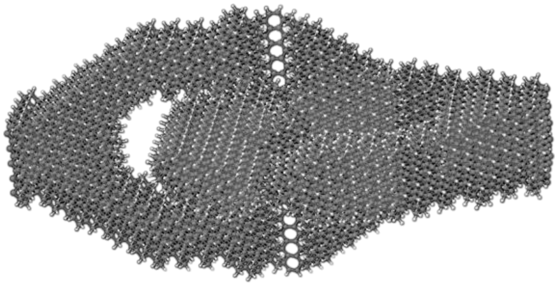
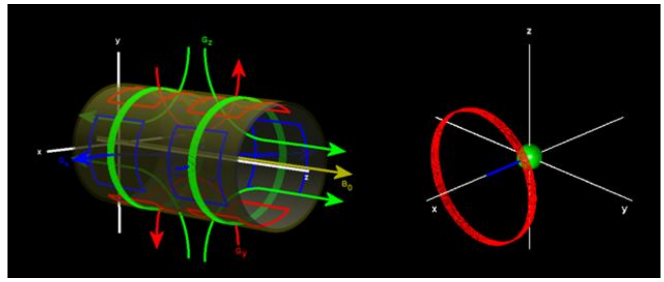


FIGURE 7
A DEPICTION OF A UNIVERSAL JOINT MADE OF CARBON AND HYDROGEN ATOMS [10]

Applications

Discussing applications of nanotechnology in the classroom is vital. Too often theory is covered without establishing a link to its influence in applications. The NanOU website has shed some light on current applications. The website focuses on three key areas of applications: medicine, alternative energy, and electronics. Arguably the most important applications occur in medicine. Figure 8 shows the structure of an MRI machine with some of the electromagnetic coils and corresponding magnetic fields. Figure 8(b) shows a single electron with its magnetic moment perpendicular to detection coils. Movement of the magnetic moment creates an induced current which ultimately will be use to create 2D images. Figure 8, again, is part of a larger animation which shows how a typical readout signal would appear as the magnetic moment changes in time. Applying nanotechnology to the MRI process involves finding ways to enhance the movement of the magnetic moment to increase image quality. An enhanced MRI image may result in a more accurate diagnosis. Other highlighted medical applications include better joint replacements through nanomaterials and precision drug delivery. Among the first applications in electronics has appeared in computer memory. The challenges of memory involve developing dense non-volatile, low power solutions. Density refers to the number of bytes per square inch, and the non-volatility indicates that the state of the memory will not change over time. MRAM (magnetic random access memory) utilizes the phenomenon of magnetoresistance to accomplish such goals. The effect of magnetoresistance, which refers to the variance of resistance to a magnetic field, increases dramatically when materials are decreased in size to the nano-scale. Alternative energy applications are very much related to electrical properties of materials. With the increasing price of oil, focus on alternative sources such as solar cell technology has increased. Conventional silicon solar cells are not incredibly efficient and are also bulky. Some companies have created thin-film solar cells by integrating nanoparticle semiconductors into an ink solution and printing the ink on thin sheets of metal substrate. While the thin-film solar cells have yet to surpass the efficiency of silicon-based solar cells, the cost of production is much lower, and there are greater possibilities of utilizing the whole spectrum by engineering



(A) (B)

FIGURE 8
(A) BASIC STRUCTURE OF MRI MACHINE SHOWING ELECTROMAGNETIC COILS AND RESULTING MAGNETIC FIELDS AND (B) A SNAPSHOT OF AN ANIMATION SHOWING THE CHANGE IN MAGNETIC MOMENT OVER TIME [9]

different nanoparticles. Figure 9 depicts a conceptualization of a multi-junction solar cell which uses differently sized nanoparticles to absorb approach energies of the solar spectrum. One typical problem in energy conversion is energy loss due to heat. By placing higher energy absorbers on the top layer, high energy photons are prevented from heating lower energy layers and decreasing efficiency.

Lab Modules

While Matlab is useful for developing customized visual aids, it is also serves along with NanoEngineer-1 as a valuable platform in laboratory exercises. A lab exercise with NE-1 gives students valuable design experience with current simulation software. In the lab, students first become familiar with the software environment followed by the construction of simple molecules as part of a tutorial. The main focus of the exercise, however, is building, simulating, and analyzing the dynamics of a carbon-nanotube switch pictured in Figure 10(a). As voltage between the nanotube and substrate changes, the nanotube bends. The CAD interface of NE-1 is extremely intuitive and eases the learning process. While the molecular dynamics of such a system are too difficult to determine by hand, students will realize the great usefulness of computational tools such as NE-1.

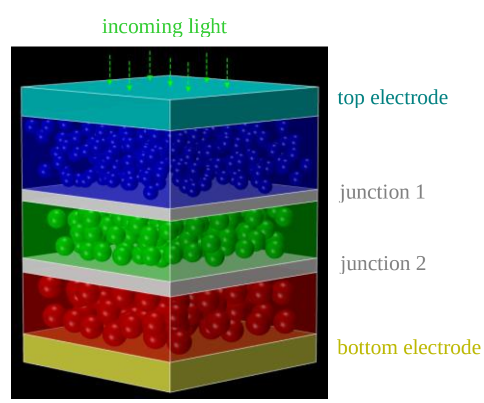
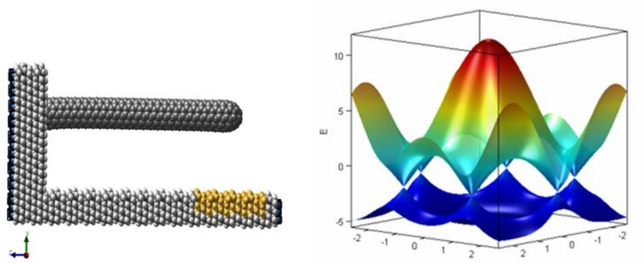


FIGURE 9
CONCEPTUALIZATION OF A MULTIJUNCTION SOLAR CELL UTILIZING TUNABLE MATERIALS TO ABSORB DIFFERENT WAVELENGTHS



(A) (B)

FIGURE 10

THE STRUCTURE OF A CARBON NANOTUBE STRUCTURE ANCHORED TO A SUBSTRATE AS MODELED IN NE-1 AND (B) OUTPUT IN MATLAB SHOWING THE ENERGY BAND STRUCTURE OF GRAPHENE

The main goals for the Matlab exercises are to introduce students to the Matlab environment as well as modeling physical aspects of nanoparticles typically used in research. For example, the energy band structure of graphene can be found from established equations in literature. The affect of atomic spacing on the results are then seen first hand. Like carbon nanotubes, graphene possesses many desirable qualities which give great potential for future applications. After a tutorial briefs students on Matlab terminology and the code implementation, students can compute the energy spectrum or band structure of graphene and develop and 3D plot of the results. Figure 10(b) gives an example of the solution.

CONCLUSION

At an involved level, conveying principles of nanotechnology is difficult because of the broad spectrum of disciplines, but these principles must be communicated in some fashion early on to show the importance of this growing field. Applications are beginning to appear and will be followed by many more in the future. Breakthroughs have already been seen in cancer research and medical imaging as well as computer memory, transistor design, and alternative energy, but many do not have a solid foundation of quantum physics to fully understand the science of nanotechnology and its applications. Being aided by various computer tools such as nanoHUB, NE-1, and Matlab provides a wide range of future possibilities for visualizing and investigating phenomena at the nano-scale. Computer-aided tools benefit people on both sides of the aisle by demonstrating concepts without having to develop new tools and by giving students experience with commonly used professional-grade, industrial programs. Combining the tools detailed in this article is an essential part of a curriculum and research plan which will bridge the gap between the disciplines or physics, engineering, biology, and chemistry. Innovative integration of supplemental material into the classroom at Oakland University has been demonstrated through a central website, NanOU.

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