EDUCATIONAL PROPOSAL: *Each applicant is expected to propose a plan that has promise to improve undergraduate science education. This is an opportunity to share the philosophy and principles that guide you as a scholar-educator. Competitive applications must include concrete examples of efforts to date, your educational plan, and how that plan supports and complements your department's undergraduate educational priorities. Your educational plan must be substantive and demonstrate a long-term commitment to your role as a scholar-educator. RCSA program officers screen educational plans/proposals initially, and only those that pass this screening are submitted to peer review of both the education and research proposals, giving equal weight to both.*

STATEMENT OF THE PROBLEM, SIGNIFICANCE OF THE PROBLEM, AND YOUR PLAN OF PROCEDURE (Describe your department's recognized areas of educational priorities and explicitly detail how your plan fits. State clearly the problems or issues you wish to address and how they relate to any ongoing work. Cite precedent. Carefully outline the importance of your plan and the impact it may have on your undergraduate students. A viable approach should be given, including examples from your own experience and/or from the literature. Indicate ways in which the completion of this work has a broader impact. Use Arial 11 point font. Limit to four pages.)

Statement of the Problem: Bolstering Inquiry-Driven Chemical Education

Many students in undergraduate chemistry curricula frequently fall back into wrote memorization and "plug-and-chug" approaches to understanding material.[51-53] Yet critical thinking, problem solving, and hypothesis-driven creative inquiry are central to scientific research, and it has been well-established that exposure to independent research experiences are highly influential in decisions to continue into graduate education.[54-57] In my experience, many students exposed to introductory general chemistry and organic courses imagine that upper level courses and research require memorizing hundreds of reactions and solving stoichiometry problems.

Computer simulations and modeling offer an important avenue towards fostering problem-solving, creative inquiry and "what-if" experiences for undergraduates that can interest them in research experiences and improve student retention. Current students are also highly computer literate and have high expectations of software interactivity derived from video games and instant messaging.[58-61] Consequently, there is a profound need for high-quality molecular builders and editors that allow free-form interactive modification with continual feedback. Students should be enabled to attempt "what-if" exercises as they build links between instructional concepts and these new interactive molecular models and simulations.

Plan of Procedure: Using Avogadro for Interactive "What If" Molecular Simulations

Previous Experience:

Like many institutions, at the University of Pittsburgh, a "Computing Across the Curriculum" effort starting in the 2003–2004 academic year sought to integrate visualization and computational modeling across all courses in the undergraduate curriculum at both the main and regional campuses. An existing off-the-shelf software package, CAChe, was adopted, and lesson plans and modules were developed to use this software to support chemical pedagogy. Results have been mixed, and no updated or new material has been produced since 2005. For example, lessons and modules do not extend to upper-level biochemistry, materials/nanoscience, or physical chemistry courses — all of which heavily rely on molecular visualization and simulation in actual research.

Beginning in the fall of 2006, before arriving at Pitt, I designed and began programming **Avogadro**,[62] an open source, freely available molecular modeling and visualization tool. While my group and myself contribute approximately half of the current development effort, the community has exploded with over 14 volunteer programmers worldwide, over 200,000 downloads, translations into over 20 languages, and adoption by many undergraduate programs and research groups alike. The software runs on Mac, Windows, and Linux, and supports the design, building, and visualization of molecules, nanoparticles, surfaces, and biomolecules.

Avogadro is *unique* in its focus around a highly interactive, intuitive program with the core goal of allowing students to easily build molecules, make free-form modification, and receive continual feedback. It integrates into many computational chemistry engines and we routinely use it in our research to edit molecules and materials, run electronic structure calculations, and visualize orbitals and other predicted properties. Because both Avogadro and many of the computational backends (e.g., MOPAC, GAMESS-US) are available free of charge, they can be used in curricular development on the undergraduate and graduate level, regardless of financial resources. The Avogadro website already provides a library of example calculations, several video screencasts, and step-by-step modules for teachers and students.

Next Steps:

As outlined above, Avogadro already has tremendous success in adoption and development of initial educational modules. In my experience, students describe the program as "video-game like," "addictive," and "easy-to-use." I wish to capitalize on this strong start with several key improvements to address the need

EDUCATIONAL PROPOSAL: *(continued)*

for creative exploration and self-discovery in the chemical curriculum. My overarching goal is to allow free-form "what-if" scenarios with Avogadro, which will help students develop from rote memorization towards deeper understanding. I believe this process improves the connection between chemical theory (e.g., VSEPR) and practical exercises for students. At the same time, they may develop an appreciation for research activities.

Understanding Dynamic 3D Molecular Structure:

In my experience, throughout the curriculum, one of the most difficult skills for students to master is relating between static, 2D images in textbooks, journals, and slide presentations and the correct, dynamic 3D shape of a molecule. At the same time, this is a key concept: the 3D shape of molecules influences reactivity and almost all molecular and material properties.

Avogadro supports "automatic optimization" of molecular geometry while drawing new bonds. Consequently, users see bond lengths, conformations, and other structural properties change quickly while the molecule changes. Such continual feedback stresses concepts such as rotational freedom, vibrations, and molecular dynamics. Avogadro also supports a "manipulation" tool, which allows students to pull or rotate individual atoms, molecular fragments or entire molecules.

Combined with the automatic optimization mode, these editing features enable students to intuitively explore intramolecular and intermolecular forces. For example, in Figure 5, the atom under manipulation is highlighted in red. For *n*-heptane, the greater rotational freedom and weaker covalent bonding enable the molecule to be stretched more easily. After students release the mouse, bonds rotate as the molecule relaxes. In comparison, pulling on an aromatic carbon atom in benzene results in less distortion and no bond rotation, because the aromatic structure is more robust. During such manipulation, the molecular model remains dynamic. Continual dragging of the mouse will pull the selected atom, and thus the rest of the molecule, across the screen.

I am building a set of lessons for both introductory organic chemistry and advanced inorganic courses around mental visualization of 2D structure depiction and the corresponding 3D shape. This will include open-ended questions where the students may alter either a 2D diagram or the 3D view in Avogadro and see the other update automatically. We will use these lessons to test concepts relating to molecular shape and function. For example, improvements will include chirality and naming for organic chemistry, and point group symmetry perception for inorganic — additional topics that will benefit from interactive learning.

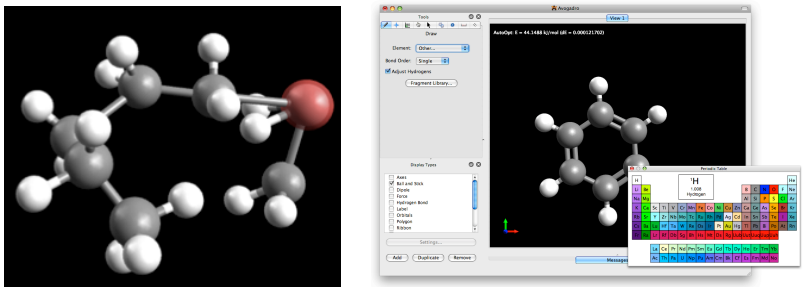

Figure 5. Interactive molecular manipulation in Avogadro. Screenshots illustrating (left) flexible *n*-heptane distorting under user manipulation and (right) rigid aromatic benzene.

Integrating Materials into Undergraduate Inorganic and Quantum Chemistry Courses:

I always strive to bring my research into the classroom. Because I frequently teach upper level undergrad courses in inorganic and physical chemistry, I build on Avogadro to develop interactive computational modeling lessons. In an effort to bring research into the classroom, I frequently discuss topics in organic electronics, conjugated polymers, and alternative energy including photovoltaics and piezoelectric materials.

Quantum mechanics is usually introduced with the particle-in-a-box model, because the equations involved are simple enough to solve exactly with basic calculus. When students progress to molecular orbital theory, the intuitive particle-in-a-box model is replaced by more advanced quantum chemical theory such as Hartree-Fock methods. For many areas of materials chemistry and nanoscience, however, the particle-in-a-box model is extremely useful. Consequently, we will introduce a module on nanomaterials after discussion of molecular orbitals. Students will begin with calculations of oligothiophenes and polyenes for discussion of the application of the one-dimensional particle-in-a-box to conducting polymer orbitals and their use in devices such as polymer solar cells and light-emitting diodes (where the HOMO-LUMO gap dictates the wavelength of emitted light). They will then continue to consider calculations of orbitals in graphene sheets (2D), C_{60} cages and gold nanoparticles (3D spheres), as illustrated in Figure 6.

EDUCATIONAL PROPOSAL: *(continued)*

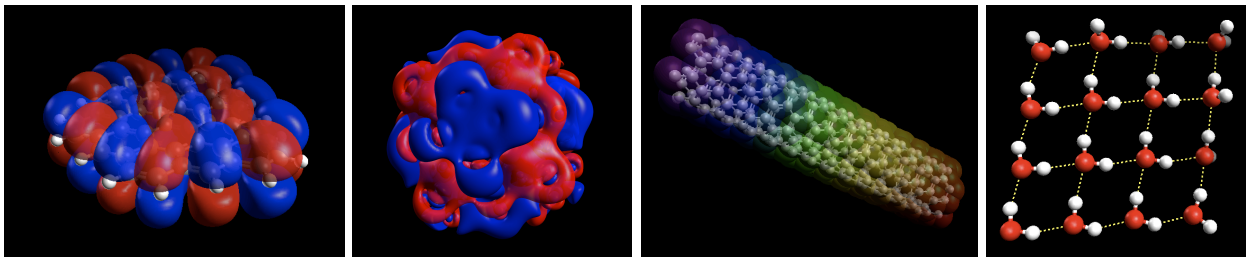

Figure 6. Examples of interactive molecular models in materials chemistry/nanoscience using Avogadro: (left-to-right) graphene surface fragment showing highest occupied molecular orbital (HOMO), gold nanoparticle showing HOMO, carbon nanotube, and hydrogen-bonded network of water molecules.

Students will be expected to perform free-form out-of-class exercises, where they test the electronic structure of nanomaterials and compare to predictions from particle-in-a-box models. Importantly, this simple model does not handle geometric distortions such as bond-length alternation in oligoacetylenes. Students will then compare with more advanced calculations including semiempirical MO calculations and density functional theory. Our goal is that students performing self-guided "what-if" experimentation will allow them move to higher levels of understanding and retention.

Embedding Web Tutorials and a Peer Forum:
Current software, Avogadro included, rely on web tutorials and exercises separate from the simulation/visualization tool. Students must either print instructions or switch between the webpages and their simulation. Instead, Avogadro will soon have an embedded web view, which will offer instruction, quizzes, and troubleshooting in the same window as the molecular view. This feature also enables us to offer a web-based peer-instruction forum for students to post questions and assist others. Most importantly, we can use web technologies to offer short pre- and post-exercise concept testing to evaluate the effectiveness of the lessons. *With funding from the Cottrell Scholar program, an undergraduate student would be hired to develop these embedded web pages, adapt existing lessons, and help build new modules.*

Impact on undergraduate research training: I strongly benefitted from undergraduate research and spent a summer in high school in an organic synthetic lab. Consequently, I have continuously had multiple undergraduate researchers in my laboratory and intend to continue this trend. Tools such as Avogadro enable me to take even lower-level students to perform computational chemistry research, and the students in my lab have enabled me to refine the interface and documentation. *Funding from the Cottrell Scholar program will enable me to support more undergrad researchers, including summer stipends.* I also seek to find talented high school students through Pittsburgh's new science and technology magnet school.

Impact on society and public education: A huge opportunity in introductory chemistry courses is the chance to impact a large fraction of future leaders in other fields. At Pitt, over 2,000 students per semester take some type of chemistry course, largely general and organic chemistry. I believe that use of interactive simulations and visualization using Avogadro can help students connect molecules to chemical research activities throughout society: biotechnology, pharmaceuticals, energy, environment, etc. Images generated using the program have already been used for book covers, posters and advertising around the world on topics such as nanoscience and biotechnology.

Other, smaller outreach activities also occur in the group. We have participated in public demonstrations at the Carnegie Museum of Natural History in Pittsburgh, including discussion of alternative energy from solar and piezoelectric sources. In graduate school, I also gave a lecture to teachers on nanotechnology and molecular electronics and found their questions enlightening. We will also organize and lead a series of lectures called "What's in Your iPod?" – explanations of the chemistry and nanoscience involved in current and new technology. For example, do students understand what happens on a basic level when attaching a wire to a battery and forming a circuit? Topics will include chemical processing in chip fabrication, charge transport in molecular materials, and applications in organic solar cells. The lecture series drives two important goals: that existing students learn to explain research to a nontechnical audience, and to recruit talented undergraduate students to pursue the research outlined in this proposal. Materials from the lecture series will be used for outreach into the K-12 schools in the Pittsburgh area.

EDUCATIONAL PROPOSAL: *(continued)*

ASSESSMENT PLAN: *Define expected outcomes of your educational plan. How will your evaluation design provide information to improve your project as it develops and progresses? How will you determine whether your stated project objectives are being met according to the proposed timeline?*

Assessment will be provided by way of student surveys of their use of Avogadro, self-assessment at understanding molecular orbital and particle-in-a-box concepts (both before and after the module), and by comparing student examination scores between two different lecture sections: one using Avogadro, and the other not.

The embedded webpage features in Avogadro will also further assessment. Students will be informed that time spent using these lessons will be recorded anonymously for research purposes. We will then compare time spent performing activities in Avogadro with improvement between the pre- and post-exercise concept questions embedded in each webpage.

Finally, our goal is that by introducing more open-ended questions and enabling students to try inquiry-driven exercises more closely aligned with chemical research, we will retain more students in the chemistry major and encourage more undergraduate research. We will test this by comparing retention rates and participation in undergrad research over the last 5 years in the department (prior to adoption of Avogadro) and over the next 3 years.

Identify departmental or institutional colleagues who might play a role in this educational endeavor (as mentors, collaborators, etc.) as appropriate and describe the role they will play.

As indicated in the attached letter from Prof. David Waldeck, the Departmental Chair, he is strongly supportive of this initiative and migrating the department's "Computing Across the Curriculum" program to adopt Avogadro across the department.

This proposal is strongly supported by Prof. Elisabeth Bell-Loncella at the University of Pittsburgh at Johnstown campus, one of the advocates for the original "Computing Across the Curriculum" initiative. She will migrate her classes, including general chemistry and inorganic chemistry to use Avogadro and modify activities accordingly. Beyond my testing and assessment of Avogadro, she will also independently assess the migration in her courses.

Prof. Ken Jordan's group heavily uses Avogadro for research purposes and we are collaborating on interactive molecular dynamics simulations for the department's physical chemistry courses, including force fields developed in his group for the accurate treatment of water.

LETTER OF SUPPORT: *Include a letter of support from your Departmental Chair, Dean or Provost that endorses your educational proposal and indicates why you are the appropriate faculty member to undertake this project. Insert this letter as Page (9a) of your application.*

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(51) Bransford, J.D.; Brown, A.L.; Cocking, R.R. *How People Learn: Brain, Mind, Experience, and School*. Washington, DC: National Academy Press, 2000.
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(54) Lopatto, D. "Undergraduate research experiences support science career decisions and active learning." *CBE Life Sci. Educ.* ***2007*** *6(4), 297.*
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