

## ACS Technology Fellowship

### Developing Molecular Simulations based courses in General Chemistry Interim progress report

Mauricio Cafiero  
Rhodes College  
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#### Summary

The purpose of this project is to design molecular simulations for use by students in General Chemistry classes. By simulating chemical phenomena and drawing their own conclusions about chemical principles, students can 'own' concepts more readily than they could in a traditional 'lecture' type setting.

#### Summer Planning

In designing the outline for a General Chemistry class featuring molecular simulations, it was decided that a mid-semester introduction of modeling techniques would work out best. I have planned a mid-semester "modeling workshop" for my students which will take up two class periods and the time in between. During this time students will learn the software, learn how to run and trouble shoot simple simulations, and make sure they have sufficient resources to use the software. After this workshop the curriculum goes into molecular structure, intermolecular forces, phase changes, and kinetic molecular theory. All of these topics are amenable to molecular simulations.

#### Planned exercises

1. **Molecular forces:** we plan to use simple exercises to show how atomic orbitals can add together to form molecular orbitals and how the squares of molecular orbitals can add together to form electron densities. We will also discuss hybrid orbitals using molecular orbital localization (this can be 'black box' to the students).
2. **Intermolecular forces:** using the electron densities we derive above we can discuss dispersion forces, hydrogen bonds, dipole moments, polarizabilities, and other density based properties.
3. **Phase changes:** the topics in (2) above can be used to discuss topics such as boiling points, lattice structures, melting points, and other phase change related topics.
4. **Kinetic Molecular Theory:** Simulations of dynamics of small clusters can be used to illustrate pressure, temperature, reaction conditions, and velocity distributions.

## **Software**

Our initial plan was to use freeware such as Tinker and Force field Explorer. A small grant obtained last year allowed us to purchase some commercial modeling software which may be more appropriate for this application. We plan to experiment using Tinker as well as Spartan and Gaussian 03. Our college is funding two student assistants who will help to test and troubleshoot these programs before we use them on our General Chemistry classes.

## **Timeline**

As the planned 'launch' of this concept is not until mid-semester, we cannot provide 'proven' materials until the end of semester. At that time we plan to submit a full report with results of student use of our modules, evaluation of the technique, and materials for use by others.

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