



**University of
Pittsburgh**

Faculty of Arts and Sciences
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To: Department of Chemistry, University of Pittsburgh
From: Michael Golde and Lisa Bell-Loncella for the CaCC
Date: 13 January 2006

As a continuation of the Computing across the Chemistry Curriculum (CaCC) initiative, we are sponsoring a workshop **Computational Chemistry for Chemistry Educators**. The workshop will run for 2½ days: all day Thursday, **March 16th**, all day Friday, **March 17th**, and Saturday morning, **March 18th**. The course will meet in the Joint Computing Classroom (JCC) located on the 3rd floor of Eberly Hall (Department of Chemistry, University of Pittsburgh, Oakland).

The course instructors will be Prof. Shawn Sendlinger (NC Central University) and Prof. Clyde Metz (College of Charleston). Additional presenters (e.g., from Gaussian) are anticipated to participate as well. The primary goal is to introduce practicing educators as well as post-doctoral fellows and graduate students interested in an academic career, to new ways to incorporate computation, modeling and molecular visualization into Chemistry courses. The workshop will be very hands-on and you will walk away with almost “ready-made” activities you can integrate into your classes. The program is not finalized, but we’ll have several areas of focus:

- Computing and molecular visualization with CAChe.
- Systems dynamics using graphical user interface differential equation solvers (GUIDES). It’s a very graphical approach to modeling physical kinetics (a classic example is the “falling calculator”) and chemical kinetics (simple first and second order chemical reaction, Michaelis-Menton kinetics and even oscillating reactions).
- Simulations – agent based modeling (good as demo material) as well as spectral simulators

The workshop presenters will provide you with a wealth of resources – most of them free and on the web. You will have an opportunity to try out all the software that is discussed in the workshop sessions. The following links may be helpful as you consider participating in this workshop:

- The Computing across the Chemistry Curriculum project (<http://chemed.chem.pitt.edu/cacc>).
- NCSI, the National Computational Science Institute (<http://www.computationalscience.org>).
- CSERD, the Computational Science Educational Reference Desk (<http://www.shodor.org/refdesk>).

The cost of this workshop will be as follows: Faculty - \$25; Post-docs & Graduate Students - \$10. There is a limit of 32 seats. In order to reserve a seat, you must submit the registration fee along with your name, title, institution, and email address to Mr. Jeffrey Palmer (412-624-5521, CSC-234; chembldg@pitt.edu). (The registration fee is non-refundable.)

Please feel free to share this invitation to other scientists at the University of Pittsburgh