



THE SHODOR EDUCATION FOUNDATION, INC.

National Science Foundation (NSF) Research Experience for Undergraduates (REU) Fellowship in Computational Quantum Chemistry

The Shodor Education Foundation, Inc. (<http://www.shodor.org>), a non-profit science and mathematics education foundation located in Durham, NC, is now **accepting applications** for a National Science Foundation "Research Experience for Undergraduates" fellowship in the area of **computational quantum chemistry**. This fellowship will provide funding during the 2001 calendar year for one outstanding undergraduate student majoring in chemistry. The position provides funding for part-time research work during the academic year, and full-time research employment during the summer. Research work is conducted both on-site at the Foundation offices in downtown Durham, and electronically via the Internet.

This fellowship will work primarily to support the ongoing development and support of the online curriculum developed for the National Science Foundation ChemViz ([http://chemviz.ncsa.uiuc.edu /](http://chemviz.ncsa.uiuc.edu/)) course.

ChemViz is a computational chemistry program that allows students to visualize molecular chemistry. Teachers and students are able to create sophisticated and accurately calculated images of orbitals and electron densities for atoms and molecules. The images are calculated using a research level program called DISCO which uses the self consistent field theory (SCF) to evaluate wave functions for electrons in the atom or molecule which is being modeled. The images and calculations are used to aid in the understanding of general, physical, and quantum chemistry.

Shodor is currently developing curriculum to support the ChemViz program. The curriculum includes informational readings, study guides, labs, and practice tests. In addition, there are various supplemental materials for educators to aid in the teaching of these concepts. The courses make use of text, graphics, and a wide variety of interactive models, animations, and Web-based calculators.

The REU fellow will work with the development team to: 1) edit current curriculum; 2) write new curriculum; 3) create additional interactive technologies, such as animations, simulations, calculators, and others as appropriate; 4) as appropriate, mentor younger interns during after-school and summer programs. The specific tasks assigned to the REU fellow will be based on the particular academic background and skill set that the

student brings. A sample task might be to write lab materials for an activity explaining basis sets. The materials would include an introduction to the lab, a background write-up briefly explaining basis sets, the lab procedure, evaluation questions, and additional activities regarding basis sets. The lab should also include relevant graphics, online calculators, example problems, and additional resources that can be found on the Internet.

Significant professional development opportunities are a key part of this fellowship, and the student will be expected to participate in other areas of the research as new skills are gained.

The ideal student for this position will be majoring in chemistry (although we are not excluding capable non-chemistry majors). In addition, the ideal student will have a solid background in math (calculus especially), a significant comfort level with computers and computing, including development of Web pages (HTML), computer programming experience (Java, perl, etc. - not as important), and other software tools (such as graphics). Applicants who are not strong in these areas are encouraged to apply, as many of these skills can be taught on-site as part of the fellowship. The ideal candidate should have outstanding communications skills, including technical writing, since a significant part of this fellowship is in developing curricular materials in the various areas. The ideal candidate should also be able to work effectively in a team environment while also being able to work independently on deadline.

Applications for this competitive fellowship are now being accepted. Applicants should submit, via email (text or attachment), the following items:

- Cover letter (email preferred)
- Current resume (email preferred)
- Two letters (emails) of support, at least one from a professor of atmospheric sciences, meteorology, earth science, or environmental science
- Anticipated availability during the academic year (it is anticipated that the student will work 5-10 hours/week during the academic year, 40 hours/week for 8-10 weeks during the summer)
- A 250-word description of experiences, career goals, and any other information that might provide "insight" into your abilities to succeed in this fellowship

All materials should be emailed to Robert R. Gotwals, Jr ("Bob2") at gotwals@shodor.org. Questions regarding this fellowship should also be addressed to this email.