Course Goals

Computational chemistry consists of two things: mathematical equations that describe molecular properties, and computer programs that implement these equations in a useful fashion. This may seem intimidating (writing a modern computational chemistry program from scratch is very difficult), but appearances are deceiving. Modern computational chemistry includes many easy-to-use tools that any chemist can use to make molecular models that are information-rich (both visually and quantitatively) and reasonably realistic.

The goal of this course is to make computational chemistry into a useful tool for you. This will be accomplished in three stages. First, you will learn how to translate chemical problems into computational problems, and how to design and perform computations that solve these problems. Second, you will learn how to analyze and interpret computational models so that you learn both the “what” and the “why” of molecular behavior. Third, you will learn about the approximations that are built into all computations, and you will learn how to remove or reduce these approximations in a systematic way. This systematic procedure can be used to validate a computational model, and it will help you choose the right type of computation for any problem. It will also help you understand why chemists perform so many different types of computations.

Course Work

The catalog describes Chemistry 324 as “lecture-computational laboratory”. In fact, most of the course takes place in the laboratory (Chemistry 105). Although I will deliver some lectures, half or more of the class sessions will be devoted to computer “experiments”. Always arrive at class promptly and ready to compute (this means completing required reading before class).

You will design some lab experiments yourself. Every student must complete 2-3 multi-week computational projects that deal with the three course goals listed above. Details concerning these projects will be handed out later in the semester.

No homework will be assigned, aside from experiments and projects. No exams will be given. Instead, I will evaluate what you are learning by monitoring the quality and thoroughness of your experimental work and the experimental reports that you write.
**We Do Not Have A Textbook**

If you have gone by the bookstore, you have learned that there is no textbook for this course. Let me explain why.

Computational chemistry has undergone (and continues to experience) explosive growth. There are many types of molecular models and there are many computer programs for generating them. No textbook (and no semester-long course) can possibly cover all of this material. A textbook writer must focus on the methods that he considers important and give short shrift to the rest. As a result, many of the excellent books that have been published on “computational chemistry” and “molecular modeling” are biased in a way that renders them unsuitable for our course. Another way to say this is, “the authors do not share my biases”.

So there isn’t any book to buy. There is material to read and learn, however. I will photocopy parts of books that I think are worth reading. You will also have to rely on lecture material and on books that you find in the library. A good starting point for pre-1997 material is the *Encyclopedia of Computational Chemistry*. This book is organized like an encyclopedia (the topics are in alphabetical order) and is kept in the reference room of the library. It does not circulate.

I can also help you find other materials. Please come see me whenever you feel like the assigned reading is unsatisfactory.

**Course Web Site**

The course home page is [academic.reed.edu/alan/324](http://academic.reed.edu/alan/324). Class announcements, such as the meeting place (Psy 102 or Chem 105), will be posted there. The course page will also contain the syllabus, copies of assignments (but not copies of the readings), and links to other some other computational web sites.