

Robert Hinde
792 Dabney Hall

rhinde@utk.edu
<http://www.chem.utk.edu/hinde.html>

Theoretical and Computational Chemistry

Students in my research group work on projects that are at the point where chemistry, physics, and mathematics meet. You might think that this sounds an awful lot like the dreaded field of *physical chemistry*, and you'd be almost completely right. It is physical chemistry, but there's really no reason to dread it. Physical chemistry is just a souped-up version of some of the things that we learn in first-year chemistry, things that are so fundamental to the field of chemistry that every chemist remembers and uses them on a near-daily basis. We're talking about ideas such as electronegativity, or "like dissolves like", or bonding and antibonding orbitals. What we do in physical chemistry is try to construct a rigorous basis for these ideas so that we can use them both to understand experimental observations and to make chemical predictions.

Our research emphasizes two main focus areas. One has to do with infrared (IR) absorption spectroscopy, which is an experimental technique used frequently in both synthetic and analytical chemistry. In an IR absorption experiment, we shine IR light on a sample to determine which wavelengths of IR light are absorbed by the sample, and what fraction of the incoming light is absorbed at each of those wavelengths. In synthetic and analytical chemistry, this is one way of determining what types of molecules are in your reaction mixture, or what the concentration is of a particular molecule in your sample. To use spectroscopy in this way, it helps to have a library of reference spectra to which you can compare your spectrum. Our goal is to try to *predict* spectra in advance — to use computers to simulate the reference spectrum of a particular molecule. We can make fairly accurate predictions of IR absorption spectra if we know how a molecule's energy and dipole moment depend on its geometry, so a lot of our effort goes into coming up with accurate ways to compute molecular energies and dipole moments.

Our group's other main focus area is in understanding the properties and behavior of low-temperature liquids and solids. When we say low temperature, we mean around 1 to 20 degrees Kelvin. We're particularly interested in understanding the properties of liquid helium and of liquid and solid H₂ at these temperatures. What's special about these two substances is that the low masses of helium atoms and H₂ molecules mean that their motions cannot be described very well using classical mechanics, so we must use quantum mechanics to really understand what's going on in these systems. But quantum mechanics gets harder and harder to apply to a system as the number of atoms or molecules in the system goes up. Sometimes we joke that a problem gets "exponentially" harder to solve when something critical happens — in quantum mechanics, that's not a joke, but a fact of life. So in our group we try to devise clever new ways to simplify or pare down quantum mechanical problems to make them small enough to tackle. Most of our projects in this broad area focus on making improvements to a simulation technique called "quantum Monte Carlo" that has a lot of potential, but also some hidden pitfalls that (we think) people haven't paid enough attention to.

All of our work falls into the broad area of computational chemistry. The molecular properties and phenomena that we're interested in are governed by the laws of quantum mechanics (remember Schrödinger's equation?) and these laws are represented mathematically by relatively complicated differential equations. We use computers to simplify the process of solving these differential equations so that we can focus on the chemical side of the problem. In our group, there are opportunities for students who would like to learn to write their own computer programs to do, especially in the second broad focus area listed above. Most of my former undergraduate researchers have entered my group without substantial computer programming experience and have learned to write their own programs as part of their research project. On the other hand, if you're pretty sure that you're *not* interested in writing your own programs, there are plenty of opportunities to carry out projects that use existing programs, particularly in the first broad focus area listed above.

What prospective undergraduate researchers in my group really need, more than anything else, is an interest in using computers in some manner to understand phenomena at the three-way intersection of chemistry, physics, and mathematics. If you think this might describe you, please e-mail me so that we can set up a time to meet each other.

Five undergraduate students in my group have received Honors B.S. degrees from UTK based on their research. These students are either now pursuing or recently completed Ph.D. degrees in chemistry at Chicago, Harvard, Princeton, and Washington State.