Cecelia Koetting, Biology

Year in School: Senior
Faculty Mentor: Dr. Rainer Glaser, Chemistry
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Molecular dynamics: Making molecules dance

During this project we took the use of the electronic structure theory in a different direction and focused on molecular mechanics use in molecular dynamics studies. By replicating many simple molecules we will later gain knowledge of the fundamental bonding theory, electron and spin densities, interactions between atoms, as well as the fundamental movements of the molecule. The computer program AMBER was used to retrieve information on how to simulate molecular motion of 10 molecules by applications of ab initio theory and of molecular dynamics methods. Aside from the numerical results, it is one of the attractive features of this project that the results led to high-quality animations. The animations produced are useful for us to learn about molecular motion. These movies help us to understand how different molecules actually move and interact with one another, as well as gain knowledge about fundamental bonding and electron and spin densities.