

Research Description

Dr. Schmiedekamp's group does calculations on molecules with transition metals surrounded by organic groups. Opportunities exist for undergraduates who have successfully completed Chemistry 110 and Math 140 to participate in these projects in computational bioinorganic chemistry. Students will learn to use programs to calculate molecular structures and energies molecules with transition metals. Some of the systems of interest are proteins with metals located in the active site. Some of the applications used are codes which implement density functional calculations (DFT) and ab initio calculations. (Jaguar and Gaussian) Other applications involve molecular mechanics and molecular dynamics calculations (CHARMM). Students will also become familiar with Linux operating systems and molecular viewers. Please see Dr. Schmiedekamp's publication list for some recent examples of projects.