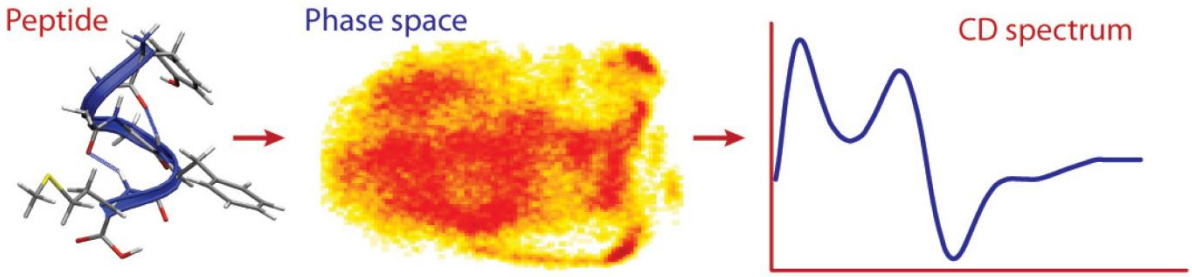
MASTER / BACHELOR PROJECTS

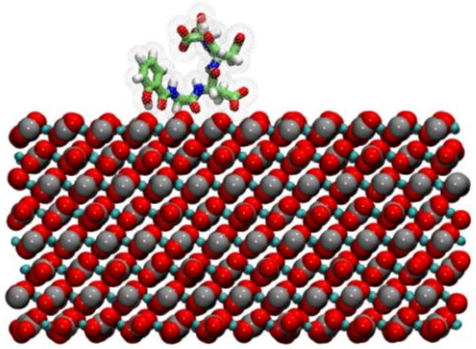
COMPUTING THE CIRCULAR DICHROISM SPECTRA OF SMALL ORGANIC MOLECULES

Circular dichroism (CD) spectroscopy is a key experimental method employed in the structural characterization of optically active chiral molecules and as such it is widely used in the studies of biologically important systems, such as peptides, proteins and DNA molecules. However, extracting useful information from experimentally obtained CD spectra can be a daunting task, especially in the case of flexible molecules. Thus, to obtain a detailed understanding of the experiments theoretical methods need to be employed.



The aim of this project is to calculate CD spectra for a range of small, biologically important organic molecules, and thereby establish a direct *molecular structure – spectrum* link. To accomplish this the student will combine state-of-the-art classical molecular dynamics simulations, which enable one to investigate the conformational properties of the molecules of interest, and advanced quantum calculations, using which CD spectra can be obtained.

THEORETICAL INVESTIGATION OF CALCITE - PEPTIDE INTERACTIONS



Many organisms produce complex, hierarchically structured inorganic materials via biomolecule-influenced crystal growth, a process known as biomineralization. Especially interesting in this respect is the mineral calcite, which is one of the most abundant minerals on the Earth's surface, and which readily interacts with small organic molecules, such as peptides, to create biominerals of interesting structural properties. However, current understanding of the interactions between biomolecules and calcite during biomineralization is far from complete. The aim of this project is to explore the mechanism of biomineralization using advanced molecular dynamics simulations, which enable one to obtain the atomistic details at the interface between biomolecules and mineral surfaces. In particular, the student will explore the interaction of small 4-residue peptides with the energetically stable surface of calcite and with a number of polar surfaces of calcite, which can play an important role in crystal growth.