Chemical Biology 4500 E 2013-2014

PROJECT ##### (NOTE THIS WILL BE ADDED LATER)

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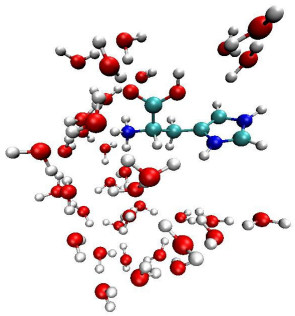
Solvation of histidine in solution and droplet environment



Solvation of aminoacids and biological macromolecules is a fundamental problem in chemistry and biochemistry as well as in related biological sciences. In this project the hydration (solvation by water) of histidine in its various charge states will be studied by using molecular simulation methods. The study will take place in two settings for comparison purposes: droplet environment and bulk solution. In the illustration a snapshot of solvation of histidine in a tiny water droplet is shown that has been modelled using quantum chemistry modelling.

The systems will be modelled by molecular mechanics force fields at the atomic level and quantum mechanical methods at the electronic level. The hydration in droplets will be characterized by solvation energies, interfacial free energies and surface tension of the droplet. In the bulk solution the effects of surface tension and interfaces do not exist, and the solvation energy due to the interactions of the solvent with the histidine will be estimated.

The students involved in the project will become familiar with methods of molecular dynamics, Monte Carlo and quantum mechanical methods used in modelling. Knowledge of computer programming is helpful but not necessary. However, the student involved in the project should be willing to learn computer programming. In the first month of the project, the student is to learn how to program and prepare a molecular dynamics code on a simple system. Then the student should be able to transfer his/her knowledge to more complex systems. Our research group has expertise in the study of chemical and physical processes in droplets and hydration of complex molecules such as macromolecules in droplet and bulk environments [see S. Consta and A. Malevanets, *J. Chem. Phys.* **138**: 044314 (2013); *J. Chem. Phys.* **138**: 184312 (2013)].