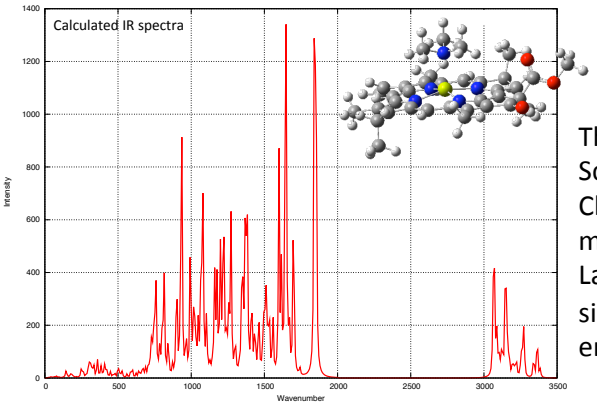
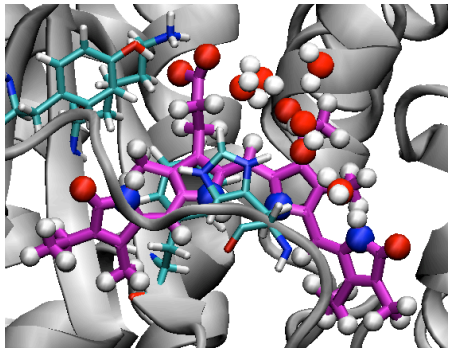
Computational Chemistry of Materials
CH455/CH752/MS508

Mon / Wed 10:10-11:55 am. Prof. David Coker



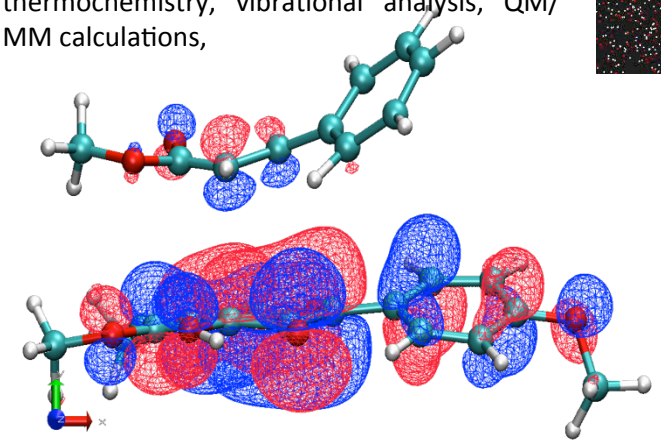
This survey course introduces GRADUATE and UNDERGRADUATE Science and Engineering students to advanced Computational Chemistry software for calculating a wide range of molecular and material properties. Lectures emphasize fundamental principles, Labs give students experience setting up and running powerful simulation codes in a high performance cluster computing environment, as well as data analysis and interpretation skills.



Electronic structure and molecular and materials simulation codes introduced: Gaussian, GaussView, NAMD, Gromacs, VMD, Antechamber and Quantum ESPRESSO and ABINIT.

Topics surveyed may include: HF SCF, LCAO-MO, basis sets, electron correlation, plane wave DFT, LDA, Kohn-Sham, exchange-correlation functionals, pseudo potentials, geometry optimization, single point energy calculations, excited states, non-radiative transitions, reaction pathways, thermochemistry, vibrational analysis, QM/MM calculations,

model potential energy surfaces, clusters, solutions and boundary conditions, MD, MC, ensembles, statistical thermodynamics, linear response, correlation functions, structure and spectroscopy, free energy calculations, meta-dynamics, enhanced sampling, Bloch's theorem, electronic and phonon band structure, Fermi surface, spin-orbit coupling, spin polarization, metals, insulators and semiconductors, projected DOS, CP ab initio MD, TDDFT, RPA, Raman, IR, absorption spectrum, optical conductivity, NEB method, many-body perturbation theory, GW, BSE, etc.…



Prerequisites: CH351 & CH352 or equivalent introductory Quantum and Statistical Thermodynamics courses approved by lecturer.

Assessment: based on lecture and computational lab assignments, final project report and presentation.

Basic computing skills: linux, editor, scripting, elementary programming, *etc.* highly useful.