Syllabus

LAB COMPONENT: building molecules; Z-matrices; internal coordinates; SCF calculations of atoms and small-to-medium sized molecules, restricted and unrestricted Hartree Fock calculations; SCF convergence criteria; geometry optimization techniques; vibrational frequency calculations and analysis of vibrational modes; calculation of Gibbs free energy of formation and Gibbs reaction energy; CI, MP2, coupled-cluster calculations of small molecules; multi-configuration SCF calculations; concept of active space; density functional calculations of large molecules; cost-benefit analysis; effects of basis sets and electron correlation - a comparison of methods; framework for crystalline solids; building crystal planes and supercells; DFT calculations of crystalline solids; simulation of molecular catalysis; biomolecular simulation using hybrid QM/MM approach.

CD61006: QMMS

Weightage:

Theory (Mid-Term and End-Term exams) - 50%

Laboratory - 50% (Includes attendance, class participation, lab reports/assignments, hands-on exercises, and/or projects)