Recent advances of theoretical chemistry

Schedule:

Theoretical chemistry, i.e. quantum chemistry and molecular modeling, play an increasingly important role in today's chemistry. The aim of the course is to introduce the student to the possibilities offered by theoretical chemistry through examples fitting his/her scientific interests, and to lay the foundations for the student to be able to communicate with theoretical chemists in the future. Therefore, after a brief introduction to the theoretical background, the student is given theoretical chemistry literature related to his/her research area to process as well as a practical assignment that he/she must complete under the guidance of the instructor.

Weeks 1 - 4: Foundations of quantum chemistry (Hartree-Fock theory, correlation methods, DFT, potential energy hypersurface, geometry optimization, solvent models).

Weeks 5 - 7: Molecular dynamics (equations of motion, integration algorithms, periodic boundary conditions, thermostats and barostats, force fields, pair correlation functions).

Weeks 8 - 12: Completing practical assignments.