CHM 624: Molecular Simulations (4)

Prerequisites: *CHM222/PHY309, CHM322/PHY303, CHM421/PHY306 or equivalent*

Introduction to scientific programming, brief overview of molecular simulation methods and their application.

Concept of phase space, statistical ensembles and averages, fluctuations, phase space distribution functions and the Liouville equation.

Born-Oppenheimer approximation, potential energy surfaces, brief overview of Hartree-Fock theory and the density functional theory, Hellman-Feynman theorem.

Description of semi-empirical **f**orce-fields and parameterization, techniques for energy minimization and normal mode analysis.

Molecular Dynamics (MD):

- Introduction to molecular dynamics, equations of motion, approximate integration schemes, force calculations, initialization and boundary conditions, potential truncation, stability, simulation of bulk phases with continuous potentials, evaluation of thermodynamic and transport properties.
- Extended Lagrangian, thermostats and barostats, methods of constraints, multiple time-steps. Methods for treating long-range Coulomb interactions, ab-initio molecular dynamics.

Monte Carlo (MC):

- Introduction, importance sampling, Markov chains and detailed balance, Metropolis method.
- Extension to various ensembles (canonical, isothermal-isobaric, grand-canonical, and Gibbs ensemble). Monte Carlo simulation of monatomic fluids and complex molecules, study of phase-equilibria.

Further Advanced Topics and Applications:

- Methods for calculation of free energy, solvation models for use with empirical potentials, advanced sampling techniques and rare events**,** combined quantum mechanical/molecular mechanical (QM/MM) methods**,** coarse-graining and mesoscale simulation methods.
- Brief introduction to commercial simulation software.

Suggested Readings **:**

- *Molecular Modelling – Principles and Applications*, A. R. Leach, 2nd Ed., Prentice Hall, 2001.
- *Understanding Molecular Simulation*s, D. Frenkel and B. Smit, 2ndEd., Academic Press, 2002.
- *Computer Simulation of Liquids*, M. P. Allen and D. J. Tildesley, Oxford,1987.
- *Essentials of Computational Chemistry: Theories and Models*, C. J. Cramer, 2nd Ed., Wiley, 2004.