Quantum Methods in Molecular Simulations (2-0-3-4)

Instructors

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Department of Chemical Engineering and Centre for Theoretical Studies

Syllabus

Analytical solution of hydrogen and hydrogenic systems; Born-Oppenheimer approximation; Formulation of Hartree-Fock method for molecular systems; Post HF methods overview; exchange and correlation concepts; configuration interaction techniques; coupled cluster technique for many-body systems; density functional theory; Exchange correlation functionals, dispersion corrections; Time-dependent DFT; geometry optimization techniques; basis sets in quantum chemistry; general framework of molecular simulations; Quantum chemical simulations of solids and crystalline materials; Simulation of molecular catalysis; vibrational analysis and frequency calculations; Simulation of molecular properties.

Lecture-wise split-up

Lecture 1-2: Analytical solution of hydrogenic systems; Born-Oppenheimer approximation

Lecture 3-4: Formulation of Hartree-Fock method for molecular systems

Lecture 5-6: Post HF methods overview; exchange and correlation concepts

Lecture 7-8: Configuration interaction techniques

Lecture 9-10: Coupled cluster technique for many-body systems

Lecture 11-12: Molecular simulation with density functional theory

Lecture 13-14: Exchange correlation functionals, dispersion corrections; TDDFT

Lecture 15-16: Quantum chemical simulation of solids; overview and solid state physics

Lecture 17-18: Quantum chemical simulations of solids and crystalline materials; Simulation of molecular catalysis

Lecture 19-20: Geometry optimization techniques; basis sets in quantum chemistry; general framework of molecular simulations

Lecture 21-22: vibrational analysis; frequency calculations

Lecture 23-24: Simulation of molecular properties

Lab component

Lab 7: Multi-configuration SCF calculations; concept of active space.

Lab 8: Density functional calculations of large molecules; cost-benefit analysis.

Lab 9: Effects of basis sets and electron correlation - A comparison of methods.

Lab 10: Framework for crystalline solids; building crystal planes and super cells.

Lab 11: DFT calculations of crystalline solids; Simulation of molecular catalysis.

Lab 12: Biomolecular simulation using hybrid QM/MM approach.

Text and References
1. Jensen F. *Introduction to Computational Chemistry*, Wiley Publishers
2. Szabo A., Ostlund N. S. *Modern Quantum Chemistry*, Dover Publishers
3. Gaussian 09, Gaussian Inc.

Exam and evaluation:
Mid-semester: 30%
End-semester: 50%
TA: 20% (term paper/presentation/simulation report)

Pre-requisites: Consent of the instructors

Maximum number of students allowed to register: 30

Semester in which the course will be offered: Spring