Computational Materials Science

Credits: 3

Lecturer:

Dr. Takahashi, Kaito
Dr. Kuo, Jer-Lai

Classroom: R311, IAMS

Class hour: Thursday, 9:10-12:00

Purpose of the course:

The goal of this class is to understand what kind of calculation is done in quantum chemistry, molecular dynamics and plane-wave based DFT package programs and to learn which method to use for the problems you want to solve! We will first learn the mathematical basics behind quantum chemistry calculations, the calculation on energies of electrons. Then we will study how these energies affect the motion of the nucleus, ie, understanding molecular structure and reaction. Next we will survey the methods used to simulate various spectra that the experimentalists take. Lastly to practice the calculation methods that was learned in class, each student will decide on a research project and perform calculation. On the final day the students will present an oral presentation on their calculation results.

Book:

(1) Modern Quantum Chemistry, Attila Szabo and Neil S. Ostlund
(2) Computational Physics, J. M. Thijssen

Syllabus:

- Born Oppenheimer Approximation, LCAO H2+ calculation
- H2, homonuclear and heteronuclear diatomic molecule, Restricted Hartree Fock.
- Unrestricted Hartree Fock, Roothan Equation, Basis Set Gaussian Calculation Input/structure optimization.
- Potential Energy Surface, Barrier Transition State.
- Electron correlation (DFT, MP2, QCISD, CCSD, CASSCF, MRCI, G2 G3)
- Vibrational Spectroscopy, Electronic Spectroscopy
- Force field parametrization, intermolecular potential
- Classical Equilibrium Statistical Mechanics (review)
- Molecular Dynamics Simulations (x2)
- Solving Schrodinger question in periodic solids (x2)
- The Monte Carlo Method
- Prepare for oral presentation
- Oral presentation

Grading:

Written exams 50% + Oral presentation/Project 50%