Computational Materials Science

Credits: 3

Lecturer:
Dr. Takahashi, Kaito
Dr. Chou, Mei-Yin
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 and solid-state physics 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.

Reference Book:

(1) Modern Quantum Chemistry, Attila Szabo and Neil S. Ostlund
(2) Materials Modelling using Density Functional Theory, Feliciano Giustino

Syllabus:

- Born-Oppenheimer approximation
- Intro on quantum chemistry calculation
- Diatomic Molecule LCAO
- Basis set, Vibration of diatomic molecule
- Hartree Fock equation
- Density Functional Theory
- Transition State Search
- Introduction to Solid-State Physics – I & II
- Introduction to Linux-based HPC
- Plane-wave based Electronic Structure Cal. – I & II
- Special Topics in Comp. Mat. Sci. – I, II & III
- Term project presentations

Grading:

Written exams/Homeworks 50% + Oral presentation/Project 50%

Week		Lecture	Subject	Hands on
1	Feb/23	K. Takahashi	General Intro Born-Oppenheimer approximation	No
2	Mar/02	K. Takahashi	Intro on quantum chemistry calculation	Electron affinity ionization
3	Mar/09	K. Takahashi	Diatomic Molecule LCAO	No
4	Mar/16	K. Takahashi	Basis set, Vibration of diatomic molecule	Simulate diatomic molecule
5	Mar/23	K. Takahashi	Hartree Fock equation	Simulate triatomic molecules
6	Mar/30	K. Takahashi	Density Functional Theory	Hartree Fock vs DFT
7	Apr/06	K. Takahashi	Transition State Search	Simulate reaction
8	Apr/13	M-Y Chou	Introduction to Solid-State Physics - I	No
9	Apr/20	M-Y Chou	Introduction to Solid-State Physics - II	No
10	Apr/27	J-L Kuo	Introduction to Linux-based HPC	Linux
11	May/04	J-L Kuo	Plane-wave based Electronic Structure Cal. - I	VASP/PWSCF
12	May/11	J-L Kuo	Plane-wave based Electronic Structure Cal. - II	VASP/PWSCF
13	May/18	TBD	Special Topics in Comp. Mat. Sci. - I	No
14	May/25	TBD	Special Topics in Comp. Mat. Sci. - II	No
15	June/01	TBD	Special Topics in Comp. Mat. Sci. - III	No
16	June/08		Term project presentations - I	
17	June/15		Term project presentations - II	