Atomistic Simulation of Materials

Introduction

Lecture 01 (2017/9/14)

School of Chem. & Mater. Sci.

ASM course

- Object: The class is aimed at beginning graduate international students and will introduce computational methods in materials science

- Instructor: Prof. Xiaojun Wu (Dept. Mater. Sci. Engi.)
  Prof. Jun Jiang (Dept. Chem. Phys.)
  Associate Prof. Wenhua Zhang (Dept. Mater. Sci. Engi.)

- Teaching Assistant: non provided, Lab will be assisted by graduate students.

- Credit: 2, lectures plus about 5 labs

- Grade: 5 problems, no final exam

- Registration: All students are required to register to obtain credits.

Topics Discussed in Course

- Why learn this course?
- Quantum Chemistry Method (2 weeks)
  - Electron & Wave Function, Schördinger Equation
  - Hartree Fock & Post Hartree Fock Method
- DFT Method (2 weeks)
  - Electron Density & KS Equation
  - LDA, GGA, GGA+U, Hybrid, Meta-GGA
- Basic Usage of Popular Software (4 weeks)
  - Gaussian, VASP, Materials Studio
- Topics in Simulations (theory & practice) (9 weeks)
  1. Model (molecule & periodic systems)
  2. Single Energy Calculations
  3. Geometric Optimization
  4. Vibration and Thermodynamic Properties
  5. Electronic Analysis (Band, DOS, Mag, WF..)
  6. Transition State
  7. How to Choose “good” Parameters?
  8. Large system calculations (MM, Semi, ONIOM)
  9. MD Simulations
  10. Introduction to Global Structure Search

Readings

- Quantum Chemistry
  - F. Jensen, "Introduction to Computational Chemistry", Wiley
  - Young D. "Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems"
- DFT
  - Koch W et al. "A Chemist's Guide to Density Functional Theory" Wiley-VCH (Basic Level)
  - Martin R. M. "Electronic Structure: Basic Theory and Practical Methods" (High Level)
- Electronic Theory
  - Sutton A P. "Electronic Structure of Materials"
  - Prasad, R. "Electronic Structure of Materials"
- Gaussian (available in USTC HPC)
  - Manual online http://gaussian.com
  - Foresman J B et al. "Exploring Chemistry with Electronic Structure Methods"
- Materials Studio (commercial)
  - Official Website http://accelrys.com
    (DMol3 references start from 2000 http://accelrys.com/products/collaborative-science/biovia-materials-studio/references/dmol3-references/index.html)
    (CASTEP references start from 2000 http://accelrys.com/products/collaborative-science/biovia-materials-studio/references/castep-references/index.html)
  - Help & Tutorial in software
- VASP (commercial)
  - Manual on Official Website https://www.vasp.at