CH121a Atomic Level Simulations of Materials and Molecules

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Prerequisites: some knowledge of quantum mechanics, classical mechanics, thermodynamics, chemistry, Unix

Introduction

Ch121a uses a practical hands-on approach for students to learn the tools of modern computational chemistry and computational materials science relevant to atomistic descriptions of the structures and properties of chemical, biological, and materials systems. This course is aimed at experimentalists (and theorists) in chemistry, materials science, chemical engineering, applied physics, biochemistry, physics, geophysics, and mechanical engineering with an interest in characterizing and designing molecules, drugs, and materials.

The lectures cover the basics of the fundamental methods: quantum mechanics, force fields, molecular dynamics, Monte Carlo, statistical mechanics, etc. required to understand the theoretical basis for the simulations while the homework applies these principles to practical problems making use of modern generally available software.

The homework each week uses available computer software implementing these basic methods on applications aimed at exposing the students to understanding how to use atomistic simulations to solve problems. This requires making decisions on the specific approaches and parameters relevant and how to analyze the results.

The final is also based on using the available software to solve problems posed to test understanding. There is a two-hour lab each week at which workstations are available for doing the homework (and exams).

Methods to be covered in the lectures include:
Quantum Mechanics: Hartree Fock and Density Function methods
Force Fields standard FF commonly used for simulations of organic, biological, inorganic, metallic systems, reactions;
ReaxFF reactive force field: for describing chemical reactions, shock decomposition, synthesis of films and nanotubes, catalysis
Molecular Dynamics: structure optimization, vibrations, phonons, elastic moduli, Verlet, microcanonical, Nose, Gibbs
Monte Carlo and **Statistical thermodynamics** Growth amorphous structures, Kubo relations, correlation functions, RIS, CCBB, FH methods growth chains, Gauss coil, theta temp
Coarse grain approaches (solvation, diffusion, mesoscale force fields beads)

Applications will include prototype examples involving such materials as:
Organic molecules (structures, reactions, diffusions);
Biochemical (amino acids, proteins, carbohydrates, nucleic acids,
Protein ligand complexes,
DNA-ligand complexes, docking);
Polymers (amorphous, crystalline, RIS theory, block);
Metal alloys (crystalline, amorphous, plasticity, dislocation).

Grading Policy:
Weekly homework 70% Final exam 30%
No Credit for late assignment.
Course homepage: http://www.wag.caltech.edu/home/ch121

Chem121a Syllabus

1. Quantum Mechanical methods and simple applications
1.1 Hartree Fock, Density Functional Theory, Configuration Interaction, Tight Binding, MNDO
1.2 Use for determining Force Fields
1.3 Use to describe Reactions

2. Force Fields methods
2.1 Energy terms: valence, van der Waals, Coulomb. Functional forms, Dreiding, UFF
2.2 Charge transfer QEq, NB Cutoffs, Splines
2.3 Obtaining Energy, Force, Hessian. Minimization: steepest descent, conjugate gradients, FP
2.4 Hessian, Normal modes, thermodynamics, dipoles, raman
2.5 MS-Q and ReaxFF force fields and their applications

3. Molecular Dynamics simulations
3.1 NVE ensemble: Newton's Equations, Verlet algorithms, time step
3.2 Velocity initialization (Boltzmann), Equilibration, Anneal, Quench
3.3 Analysis: fluctuations, Kubo, Free Energy Pert Theory
3.4 NVT ensemble: derive Nose-Hoover thermostat.
3.5 Entropy (Velocity AutoCorrelation/Wilson), Thermodynamics
3.6 NPT ensemble: fluctuation-dissipation, specific heat, compressibility, thermal expansion, viscosity.
3.7 Quantum Hopping MD

4. Monte Carlo methods
4.1 Markov, Metropolis, RIS, CCBB

5. Solvation Methods
5.1 PB, QM, MD, MC; SGB, AVGB

6. Simulations of Biological systems
6.1 Proteins: peptides, Alpha Helix, Beta Sheet, PDB, heme
6.2 ligands, Dock, HierDock
6.3 DNA: B, Z, A,sugar, PO4, ligands,Amber, Charmm
6.4 Membrane Prot, lipid; united atom, Calpha

7. Simulations of crystalline systems
7.1 Crystal classes, optimizations of cell paramters.
7.2 Phonons (acoustic, optical), Brillouin zone.

7.3 Elastic constants, Young, Poisson, vel. Sound
7.4 Methods for simulations with periodic boundary condition: XQEq, Ewald, CMM, splines
7.5 Metals: Metallic FF, Finnis, EAM, qEAM
7.6 Periodic QM calculations (SeqQuest,CasStp, Dmol-3D, Crystal)
7.7 Crystalline polymers (PE, Nylon, PVDF)
7.8 FH, Gauss coil, theta temp, amorphous, CED, SP, PTFE,Co-Polymers

8. Optical properties: time dependent DFT, refractive index

9. Modeling of dynamical processes: rare events
9.1 Transition States, VTS, unimolecular reactions, RRKM,
9.2 Diffusion
9.3 Kinetic Monte Carlo

10. Nanotechnology
10.1 Nanoelectronics: Rotaxanes
10.2 Fullerenes, bucky tubes
10.3 AFM Nanoprobes

11. General applications
11.1 Sugars, Carbohydrate, atomistic and coarse-grained simulations
11.2 Boron diffusion in Silicon
11.3 Dislocations in metals, single crystal plasticity
11.4 Superconductors: structures, properties, and mechanisms.
11.5 Ceramics: structures, properties, and phase transitions.
11.6 Organic force fields: OPLS, MM3.

Organized by Lectures

1. WAG intro- closed shell HF, DFT, basis sets
2. Trans. States, vibration; CI, tight binding, mndo
3. Reactions.QM (metathesis, polymerization),VTS
4. FF: Valence, vdw, coulomb:Dreiding, UFF, Amber, Charmm,MM3,OPLS
5. QEq, NB Cutoffs, splines
6. ReaxFF, applications to HE, MoOx,Si/SiO2, catalysts, nanotech
7. QM-->FF --> E, Force, Hessian;Minimize: SD, CG, FP
8. Hessian, Normal modes, dipole, raman, Thermodynamics
9. NVE: Newton's Eqn, Verlet(x,v), Boltz dist, Equil., Anneal, Quench
10. NVT: derive Nose-Hoover, tau;NPT, Andersen, Rahman-Parrinello
11. Entropy (VAC/Wilson), Thermodynamics, liquids, diffusion
12. Markov, Metropolis, RIS, CCBB, FH, Gauss coil, theta temp
13. amorphous polymers, surface tension, IFT
14. PB, SGB, AVGB,COSMOS: neutrals and ions
15. Proteins: peptides, Alpha Helix, Beta Sheet, PDB --> MD
16. Homology, Sequence to Structure, Ca FF, Amber, Charmm
17. Ligand binding, Dock, HierDock

18. GPCR: structure and ligand binding
19. DNA: B, Z, A,sugar, PO4, ligands,
20. cell coord, opt. Cell, Ewald, elastic constants, Youngs modulus
21. Metallic FF: FS, SC, EAM, qEAM,dislocations, plasticity
22. polymer crystal (PE, Nylon, PVDF)
23. QM-PBC (SeqQuest,CasStp, Dmol-3D, Crystal), Car-Parrinello:Al appl.
24. Diffusion (protons, molecules), QHMD
25. nanotechnology, fullerenes, bucky tubes, Rotaxanes
26. NEMD, viscosity, Green-Kubo,fluctuations, Cp,comp, thermal expan,
27. sugars, Carbohydrate, atomistic and beads, diffusion