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Molecular Modeling of Aqueous Solutions and Substrate-Solution Interfaces  

Spring Semester 2007  

GEOL 593-J2 is a review course that introduces methods and techniques of computational molecular modeling and their application to the fundamental understanding of the atomic- and molecular-level origins of physical and chemical properties and processes related to water purification and desalination.

The course is intended for graduate students (associated with the WaterCAMPWS or not) who have relatively limited background in theoretical thermodynamics, statistical mechanics, molecular materials science, and computer programming, etc., essentially those who are perhaps doing mainly experimental research, but who still need and desire to know and understand at least some basics of molecular modeling approaches in order to better understand the current literature on the subject. About 20 recent research papers on molecular modeling of interfaces, membranes, etc., are prepared for discussion during the course.

In contrast to the course initially offered in the Spring Semester 2005, this time the course spans not half a semester (1 credit hour), but the entire semester (4 credit hours) and includes not only lectures-discussions, but also hands-on computer exercises using the VizLab facilities and the computational materials chemistry software (Cerius2 and Materials Studio) available at the School of Chemical Sciences, UIUC.

Syllabus

- Brief introduction to statistical mechanics  
  - Mechanical state vs thermodynamic state of a system; partition function  
  - Macroscopic properties of materials from statistical mechanics  
  - Ergodicity; time averages vs ensemble averages  
- Monte Carlo (MC) molecular computer simulation techniques  
- Molecular dynamics (MD) computer simulation techniques  
- Periodic boundary conditions  
- Intermolecular potentials (force fields) for simulation of aqueous systems  
  - Molecular models of water; ab initio vs empirical potentials  
  - Many body interactions  
  - Hydrated ions  
- Calculation of macroscopic properties from MC and MD simulations  
  - Thermodynamic properties  
  - Fluid structure; radial distribution functions (RDFs)  
  - Mean square displacement (MSD) and self-diffusion coefficients  
  - Velocity autocorrelation functions (VACFs)  
  - Power spectrum (density of states) of atomic motions  
  - Dielectric properties
• **Hydrogen bonding in aqueous systems**
  o Geometric, energetic and other criteria of H-bonding
  o Donating and accepting H-bonds; local tetrahedrality of water structure
  o Statistical analysis of H-bonding
  o Variations of H-bonding with thermodynamic state conditions and local molecular environment

• **Interfaces of aqueous solutions with inorganic substrates**
  o Molecular models of inorganic membranes
  o Rigid vs flexible substrate
  o Structure, energetics, and dynamics of aqueous interfaces and interlayers
  o Hydrophobic and hydrophilic surfaces
  o Local electrostatic fields and orientation of surface H₂O molecules

• **Computational modeling of polymer membranes for water purification and desalination**
  o Molecular models of polymer membranes; polyamide membranes for reverse osmosis
  o Modeling of variable protonation states of polyamide membranes
  o Ionic hydration and transport of H₂O and ions in polyamide membranes

• **Adsorption of metal cations to natural organic matter (NOM)**
  o Molecular models of NOM (humic acid)
  o Interaction of metal cations with NOM: Structure, energetics and dynamics

**The exercises include:**

  o building the models of aqueous interfaces for molecular modeling:
    Á aqueous salt solutions
    Á aqueous NOM solutions
    Á molecular models of inorganic (mineral) interfaces
    Á molecular models of polymer membranes and membrane-water interfaces

  o selecting force fields for molecular simulations

  o molecular mechanics, energy minimization and structure optimization techniques

  o preparing input parameters for molecular dynamics simulations of the selected systems

  o running MD simulations of the selected systems

  o quantitative analysis of the MD computer simulation results
    Á thermodynamic properties of aqueous solutions and interfaces
    Á structure of aqueous solutions in the bulk phase and at the interfaces
    Á diffusion of aqueous species
    Á velocity autocorrelation functions and power spectra of atomic motions in aqueous solutions in the bulk phase and at the interfaces
    Á atomic density profiles and surface density maps of aqueous species from interfacial simulations
Literature

Textbooks (none is specifically required, but these two are recommended):


Some other useful textbooks:

3) Alan Hinchliffe “Molecular Modeling for Beginners”, John Wiley & Sons Ltd, 2003, 410pp. (recommended)

Research papers:


