CHM1485: Molecular Dynamics and Chemical Dynamics in Liquids

Location: University College, Room 330
Dates and Time: Tuesdays, 3:00 pm - 5:00 pm

Instructors

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Grading

1. 4 problem sets 70%
2. Short litterature report (12 page limit) 30%

TOPICS COVERED

1. Review
    - Classical Mechanics
    - Ensembles
2. Basic properties of liquids
    - Physical characterstics
    - Phase diagrams
    - Basic models
3. Statics and phase transitions
    - Distribution functions
    - Density functional theory
4. Stochastic models
    - Random walk and Brownian motion
    - Fokker-Planck equation and Kramer's problem
5. Microscopic transport
    - Self-diffusion
    - Chemical kinetics
    - Hydrodynamics
6. Simulations
    - Monte-Carlo
    - Molecular dynamics: thermostats
7. Liquids out of equilibrium

Suggested Reference Books:

- "Statistical Mechanics", by Donald A. McQuarrie
- "Statistical Physics: Statics, Dynamics and Renormalization", L.P. Kadanoff
- "Theory of Simple Liquids", J.-P. Hansen and I.R. McDonald
- "Basic Concepts in Complex and Simple Liquids", Barrat and Hansen
- "Understanding Molecular Simulation", Frenkel and Smit
- "Stochastic Processes in Physics and Chemistry", N.G. van Kampen