MAT 306 Computational Techniques for Materials at the Nano-scale

Spring 2021

Intended Audience:
A junior level hands-on course for MAT, BIO, and CS majors, PHYS and CHEM minors, or anyone who would like to roll up her/his sleeves for modeling materials and obtain their characteristic properties "in silico."

Objective:
The goal of this course is to introduce various modeling techniques operative at a broad range of time and length scales relevant to the understanding of the structure-property relationships of "materials" where a material is defined in the broad sense of anything that is utilized for a particular human defined purpose; to introduce a conceptual framework for the understanding of macroscopic observations of materials from a microscopic viewpoint.

Moderator:	*Name:*	Ali Rana Atılgan
	Office No.:	FENS 2093
	Phone No.:	+90 (216) 483 9525
	e-mail:	atilgan@sabanciuniv.edu
	URL:	http://people.sabanciuniv.edu/atilgan
Associate:	Dr. T. Fürkan Güçlü	furkan.guclu@sabanciuniv.edu
Learning Assistant:	Defne Çirci	defnecirci@sabanciuniv.edu
Course Data:	Hours/Class	Mon 08.40-10.30; Tue 08.40-09.30/FENS G055
	Office hours:	*TBA*

Textbook:

Leach, A.R., *Molecular Modelling*, 2nd Ed. Prentice Hall, 2001. ISBN: 0-582-38210-6

References:

Hinchliffe, A., *Molecular Modeling for Beginners*, 2nd Edition. Wiley, 2008. ISBN: 978-0-470-51314-9

Weeks Commencing/Topics:

Feb 28 and Mar 7
The problem of time and length scales in molecular modelling; molecular graphics.
Useful concepts in molecular modeling: Coordinate systems; potential energy surfaces; degrees of freedom

Mar 14 and 21
Force fields and how to get a simple potential energy surface from a simple molecular dynamics (MD) run
Calculating potential of mean force from MD simulations

Mar 28 and April 4
How to extract barrier heights between the different conformations of a molecule
Energy minimization; non-derivative, first derivative and second derivative methods.

Apr 11 Review and **Exam I**

Apr 18
Normal mode analysis

Apr 25 and May 9
(**May 2** Spring Break)
Ingredients of an MD simulation
- the Verlet algorithm; choosing the time step
- conservation of energy; controlling the temperature

May 16 and 23
Thermodynamic properties that may be calculated via MD simulations
Calculation of kinetic properties from an MD simulation

May 30 Review and **Exam II** (two parts, in-class and take home)

June 6 Presentations of Take Home Exam II

Software

NAMD and VMD both of which may be reached at http://www.ks.uiuc.edu/

Learning objectives

Interpret the problem of time and length scales in molecular modeling by relating the type of the problem to the available modeling technique;

Sketch simple potential energy surfaces for systems of up to four particles and identify the global energy minimum and local energy minima on it;

Calculate the energy of conformations of simple molecules of up to six particles, given the parameters of a force field describing the molecule;

Relate the influence of conformations of a molecule on its properties by calculating the average properties of a given system based-on the Boltzmann distribution;

Perform conformational searching on systems by applying systematic and random search methods;

Perform normal mode analysis on systems in one and two-dimensions and relate the output to vibrational spectroscopy experiments;

Set-up and run molecular dynamics simulations on complex systems such as polymers and proteins;

Make physics-based descriptions of the main ingredients of a simulation such as the Verlet algorithm, periodic boundary conditions, selection of time step;

Calculate thermodynamic (*e.g.,* temperature, pressure, heat capacity), and kinetic properties (diffusion constant, various relaxation times) from simulated trajectories.

Class Policies

Course will be hybrid.

Zoom link:

https://sabanciuniv.zoom.us/j/94354668055

Grading

Assignments: (5 of them), total is for 50% of the final grade

Interim exam: (2) each 25% of the final grade