

Selected Topics in Physical Chemistry: Introduction into Computational Chemistry CHEM 5570-101 (Fall 2022)

Times: T/R 09:30am to 10:50am (until 9/22)

Location: SLSRC 2430

Course Instructor: Dr. Ulrich H.E. Hansmann

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Office hours: T/R after class or by appointment

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Course web site: <http://hansmann-lab.com/cbpc/hansmann/5570.php>

Description

The purpose of this course is to introduce fundamental concepts of quantum mechanics and statistical mechanics and their application to molecular simulations and structure prediction. No programming skills are required. The course is directed toward graduate and advanced undergraduate students in physical chemistry, biochemistry, bioengineering and chemical engineering. The following concepts will be discussed:

- 1) Role of computers in chemistry and structural biology (structure prediction, analysis and interpretation of experimental data, augmentation of experiments)
- 2) Concepts of simulations and modeling (models, energies and forces, dynamics versus thermodynamics; introduction into statistical mechanics)
- 3) Quantum Mechanics and energy calculations
- 4) Force fields
- 5) Monte Carlo sampling
- 6) Molecular Dynamics
- 7) Enhanced sampling techniques
- 8) Free energy calculations
- 9) Example: simple molecular dynamics simulations using GROMACS
- 10) Example: evaluating binding sites using AutoDock.

Pre-requisites

Undergraduate-level Physical Chemistry and Calculus I and II required.

Textbooks

- M .P. Allen and D. J. Tildesley, "Computer Simulation of Liquids". Oxford

- University Press, 1987.
- A. R. Leach, "Molecular Modeling", Prentice Hall, Second Edition, 2001.

Grading Scheme

Home work: 100%

Home work extensions

Assignment deadline extensions will be given only under extreme circumstances and only with prior notification and documentation. There will be no extra credit assignments given.

University codes and policies of behavior

See "University policies regarding instruction" downloadable from the Provost's website,

<http://www.ou.edu/provost/pronew/content/memorand.html>

Each student should acquaint her or his self with the University's codes, policies, and procedures involving academic misconduct, grievances, sexual and ethnic harassment, and discrimination based on physical handicap.

Any student in this course who has a disability that may prevent him or her from fully demonstrating his or her abilities should contact me personally as soon as possible so we can discuss accommodations necessary to ensure full participation and facilitate your educational opportunities.

Academic Misconduct

Any form of academic misconduct, as specified in the Student Code at OU and in the Chemistry Department's Graduate Student Handbook, will be reported to the Department and the Dean for appropriate action.

Other notes

I reserve the right to change by addition and/or subtraction any and/or all materials contained in this syllabus. This includes, but is not limited to, course content, assignments, due dates, and portion(s) of the grade assigned to individual items within this course.