KJM5630 – Multi-scale molecular modelling

Note: the text is a modified version of the current description.
Red: new text, ~~**strikethrough:**~~ removed text.

Course content

The course is designed to give students in chemistry and related subjects an introduction to the theory for molecular modeling, and use of modeling as a ~~**tool**~~ fundamental conceptual approach in ~~**chemical**~~ molecular-based research. Considerable emphasis will be placed on practical use of modeling and an understanding of the methods which extends beyond purely operational skills. The aim is to give the students the sufficient background to independently evaluate choice of methods and reliability of results in molecular modeling.

Learning outcome

When you have completed this course, you can

- Understand the theoretical connection between statistical and quantum mechanics, and computer modelling.
- Understand how macroscopic thermodynamic quantities, including free-energy profiles or reaction rates, can be derived from microscopic mechanical properties
- Understand how ~~**quantum mechanical models**~~ molecular models at different scales and resolutions can be used to describe ~~**chemical reactions and properties**~~ different (bio)chemical and (bio)physical phenomena
- Master the fundamental algorithms used in molecular modeling, including molecular dynamics, and Monte Carlo, as well as more advanced enhanced sampling techniques. (THIS IS ADDED IN PARTICULAR THINKING TO CS STUDENTS).
- Explain strengths and weaknesses of different models (~~**molecular mechanics, semi-empirical, wavefunction based and density functional theory**~~ including ab initio, molecular mechanics, QM/MM, coarse grained, and mesoscale)
- ~~**Explain how quantum mechanics can contribute to the understanding of reaction mechanisms in organic chemistry and catalysis.**~~
- Evaluate the accuracy of performed calculations
- Present results from computational studies in both oral and written form

Admission

Students who are admitted to study programmes at UiO must each semester register which courses and exams they wish to sign up for in Studentweb.

Students enrolled in other Master's Degree Programmes can, on application, be admitted to the course if this is cleared by their own study programme.

If you are not already enrolled as a student at UiO, please see our information about admission requirements and procedures.

Prerequisites

Recommended previous knowledge

KJM2600 – Physical chemistry II - quantum chemistry and spectroscopy.
KJM4XXX (the substitute of KJM-MENA3300)
Basic Maths
Basic Programming
~~**A minimum in mathematics corresponding to MAT1001 – Mathematics 1 (discontinued)**~~

Overlapping courses

- 10 credits overlap with KJM9630 – Multiscale molecular modelling (change of title accordingly)
- Sjekk overlapp mot tidligere emner som KJM3600 og KJM4600.

Teaching

The course consists of 30 hours of lectures and 32 hours of computer lab (eight sessions). During the computer lab, students will develop a code that will be used both during classes, and for the final examination. The final examination will consist of a do-at-home project, and a final oral evaluation.

The project is valid only the semester it is assigned.

The first lecture and the computer labs are mandatory.