Institutionen för organisk kemi

Stockholms universitet

Kursplan

för forskarkurs

Theoretical Organic Chemistry **15.0 Högskolepoäng**

Theoretical Organic Chemistry **15.0 ECTS credits**

Kurskod:	KO40006
Gäller från:	VT 2020
Institution	Institutionen för organisk kemi

Förkunskapskrav och andra villkor för tillträde till programmet

Admitted to PhD studies

Lärandemål

At the end of the course the students will be able to:
- Use standard quantum chemistry packages, such as Gaussian.
- Perform advanced calculations on chemical structures and reactions.
- Formulate strategies for modelling chemical reactions and define appropriate ways to test the adequacy of the models.
- Rationalize organic/organometallic reactivity and selectivity on the basis of calculations.
- Critically examine computational chemistry research paper in the organic chemistry literature.

Innehåll

Computational chemistry is today an indispensable tool in essentially all branches of chemistry. In particular, quantum chemistry has proven very valuable in the fields of organic and organometallic chemistry, where it has had a major impact. Continuous development of the underlying theories and techniques, together with the exponential growth of computer power, have led to a very rapid advancement of the field and have made it possible to achieve high accuracy at a reasonable computational cost.

The course is aimed at experimental organic chemists intending to use quantum chemical modeling in their research. It involves both quantitative and qualitative aspects of quantum chemistry focused on organic and organometallic applications.

Specific aims of the course are:

i) to introduce the field of computational chemistry to graduate students in organic chemistry in such a way that it becomes one of their standard tools in their research activities.
ii) to give advanced knowledge on models and concepts used to describe chemical structure and reactivity.
iii) to give insight into mechanistic features of organic/organometallic reactivity using quantum chemical approach.

The course consists of the following parts:

i) Basic theory, covering the following aspects:
- The Hartree-Fock (HF) method

- The linear combination of atomic orbitals (LCAO) method
- Basic density functional theory (DFT)
- Basis sets
- Geometry optimization
- Potential energy surfaces and their interpretation
- Solvation methods
- Dispersion interactions
- Calculation of thermal corrections
- Transition state theory (TST)
- Microkinetic modeling
- Basic force fields and molecular mechanics (MM)
- Basic molecular dynamics (MD) simulations

ii) Computer exercises introducing the various technical elements of the calculations step by step such that at the end the student will be able to run advanced calculations on realistic problems.
The following topics are covered:
- Basic Linux commands
- The GaussView software for building and visualizing molecules
- Benchmarking of computational methods
- Optimizing transition states of chemical reactions
- Solvation calculations
- Calculation of pKa values
- Calculation of dispersion correction
- Cycloaddition reactions
- SN2 reactions
- Oxidative addition / reductive elimination reactions
- Metal-catalyzed C–H functionalization reactions

iii) Individual project, where the students can choose to focus on a specific topic from their research if they want.

Obligatoriska moment

Participation in computer exercises is mandatory.

Examinationsformer

The course is examined as follows:
a) Written examination of the theory part.
b) Written reports on the computer exercises.
c) Written report on the individual project and an oral presentation of the obtained results.

Grading of all three parts is conducted according to a two-point grading scale: Pass or fail. The grading criteria are communicated and explained at the start of the course.
Students who fail in the regular exams are entitled to write further exams as long as the course is given. The number of test occasions is not limited.

Arbetsform

The teaching consists of lectures, computer exercises, and a supervised research project.
The teaching is conducted in English.