Chemical Bonding, 6.0 credits

Kemisk bindning, 6.0 hp

Third-cycle education course

6FIFM82

Department of Physics, Chemistry and Biology

Valid from: Second half-year 2025

Approved by **Approved**

Registration number

Entry requirements

Entry requirement for studies on third-cycle education courses

- second-cycle degree,
- 240 credits in required courses, including at least 60 second-cycle credits, or
- acquisition of equivalent knowledge in some other manner

Specific information

The target group is doctoral students who have obtained a second-cycle degree in chemistry, molecular physics, or an equivalent field.

Learning outcomes

By the end of the course the students will be able to:

- Demonstrate knowledge and understanding by giving accounts of elementary quantum mechanical theory and how this can be applied to infer quantization and the concept of orbitals and to execute quantum chemical calculations
- Use molecular orbital theory to explain the electronic structure of molecules
- Describe chemical bonding starting from molecular orbital theory
- Discuss various forms of chemical bonding and their relevance for the properties of substances
- Show competence and skills by performing simple computer based molecular modelling
- Apply concepts of symmetry to classify molecular geometries, orbitals and vibrational modes and to explain the appearances of electron excitation spectra and vibrational spectra.

Judgement and approach are conveyed by raising awareness of theoretical modeling as a complement to or substitute for other experimental activities.

Contents

The course cover how the electronic structure and geometry of molecules can be obtained from the results of the elementary theory of quantum mechanics, and how molecular properties are reflected in the electronic and structural properties of various materials. The course discusses chemical bonding starting from the concept of molecular orbitals and rationalizes the shape of orbitals and spectra from infrared and Raman spectroscopy starting from symmetry considerations, plus conveys proficiencies in operating modern molecular modeling tools.
Quantum mechanics: the Schrödinger equation, energy quantization, wave functions, the hydrogen atom, atomic orbitals, orbital energy diagrams
Quantum chemistry: diatomic molecules, molecular orbitals, the types of chemical bonding covalent bonding, polar covalent bonding and ionic bonding, larger molecules, the Hückel approximation, computational chemistry
Symmetry: symmetry operators and symmetry elements, classification of symmetries, point groups, character tables, applications on molecular orbitals, electron excitation spectroscopy and vibrational spectroscopy
Laboratory course where molecular modelling is performed, and vibrational spectra are examined.

Educational methods

The educational methods in this course include lectures, lessons, and laboratory sessions

Examination

Assessment is based on a written examination and two laboratory reports. Attendance at the laboratory sessions, completion of the experiments, and approved laboratory reports are mandatory to pass the course.

Grading

Two-grade scale

Course literature

The course literature includes the textbook Peter Atkins, Julio de Paula, James Keeler: Atkins' Physical Chemistry, Oxford University Press, and the scientific article Emma M. Björk et al., Formation of block-copolymer-templated mesoporous silica, Journal of Colloid and Interface Science 521/2018/183–189, https://doi.org/10.1016/j.jcis.2018.03.032, as well as laboratory instructions. Supplementary course literature is Yves Jean, François Volatron: An Introduction to Molecular Orbitals, Oxford University Press

General information

The course is planned and carried out according to what is stated in this syllabus. Course evaluation, analysis and suggestions for improvement should be fed back to the Research and PhD studies Committee (FUN) by the course coordinator.