

# Chemical Bonding

Programme course

6 credits

Kemisk bindning

NKED22

Valid from: 2019 Spring semester

**Determined by**

Board of Studies for Chemistry, Biology  
and Biotechnology

**Date determined**

2018-08-31

## Main field of study

Chemistry

## Course level

Second cycle

## Advancement level

A1X

## Course offered for

- Master's Programme in Chemistry

## Entry requirements

Note: Admission requirements for non-programme students usually also include admission requirements for the programme and threshold requirements for progression within the programme, or corresponding.

## Prerequisites

Bachelor of Science program in Chemistry

## Intended learning outcomes

The course is intended to convey basic knowledge on 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 is intended to provide the student with tools to enable the discussion of chemical bonding starting from the concept of molecular orbitals and to rationalize the shape of orbitals and spectra from infrared and Raman spectroscopy starting from symmetry considerations, plus to convey proficiencies in operating modern molecular modeling tools. At the end of a successfully completed course the student is intended to be able to:

- Give an account 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 materials
- Explain how the electric properties of materials originate from their electronic structure
- Execute simple computer based molecular modelling
- Apply concepts of symmetry to classify molecular geometries, orbitals and vibrational modes and to explain the appearances of vibrational spectra.

## Course content

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

Crystals: different types of crystal bonding such as covalent network bonding and metal bonding, crystal structure, X-ray and neutron spectroscopy, band theory

Laboratory course where molecular modelling is performed, and vibrational spectra are examined.

## Teaching and working methods

The course consists of lectures, lessons and laboratory work.

## Examination

LAB1	Laboratory work	2 credits	U, G
TEN1	Written examination	4 credits	U, 3, 4, 5

## Grades

Four-grade scale, LiU, U, 3, 4, 5

## Department

Institutionen för fysik, kemi och biologi

## Director of Studies or equivalent

Magdalena Svensson

## Examiner

Lars Ojamäe

## Education components

Preliminary scheduled hours: 46 h

Recommended self-study hours: 114 h

## Course literature

### Books

Peter Atkins and Julio de Paula, *Atkins' Physical Chemistry* Oxford University Press

Yves Jean François Volatron, *An introduction to molecular orbitals* Oxford University Press

## Common rules

### Course syllabus

A syllabus has been established for each course. The syllabus specifies the aim and contents of the course, and the prior knowledge that a student must have in order to be able to benefit from the course.

### Timetabling

Courses are timetabled after a decision has been made for this course concerning its assignment to a timetable module. A central timetable is not drawn up for courses with fewer than five participants. Most project courses do not have a central timetable.

### Interrupting a course

The vice-chancellor's decision concerning regulations for registration, deregistration and reporting results (Dnr LiU-2015-01241) states that interruptions in study are to be recorded in Ladok. Thus, all students who do not participate in a course for which they have registered must record the interruption, such that the registration on the course can be removed. Deregistration from a course is carried out using a web-based form: [www.lith.liu.se/for-studenter/kurskomplettering?l=sv](http://www.lith.liu.se/for-studenter/kurskomplettering?l=sv).

### Cancelled courses

Courses with few participants (fewer than 10) may be cancelled or organised in a manner that differs from that stated in the course syllabus. The board of studies is to deliberate and decide whether a course is to be cancelled or changed from the course syllabus.

### Regulations relating to examinations and examiners

Details are given in a decision in the university's rule book:  
<http://styrdokument.liu.se/Regelsamling/VisaBeslut/622678>.

### Forms of examination

#### Examination

Written and oral examinations are held at least three times a year: once immediately after the end of the course, once in August, and once (usually) in one of the re-examination periods. Examinations held at other times are to follow a decision of the board of studies.

Principles for examination scheduling for courses that follow the study periods:

- courses given in VT1 are examined for the first time in March, with re-

examination in June and August

- courses given in VT2 are examined for the first time in May, with re-examination in August and October
- courses given in HT1 are examined for the first time in October, with re-examination in January and August
- courses given in HT2 are examined for the first time in January, with re-examination at Easter and in August.

The examination schedule is based on the structure of timetable modules, but there may be deviations from this, mainly in the case of courses that are studied and examined for several programmes and in lower grades (i.e. 1 and 2).

- Examinations for courses that the board of studies has decided are to be held in alternate years are held only three times during the year in which the course is given.
- Examinations for courses that are cancelled or rescheduled such that they are not given in one or several years are held three times during the year that immediately follows the course, with examination scheduling that corresponds to the scheduling that was in force before the course was cancelled or rescheduled.
- If teaching is no longer given for a course, three examination occurrences are held during the immediately subsequent year, while examinations are at the same time held for any replacement course that is given, or alternatively in association with other re-examination opportunities. Furthermore, an examination is held on one further occasion during the next subsequent year, unless the board of studies determines otherwise.
- If a course is given during several periods of the year (for programmes, or on different occasions for different programmes) the board or boards of studies determine together the scheduling and frequency of re-examination occasions.

### **Registration for examination**

In order to take an examination, a student must register in advance at the Student Portal during the registration period, which opens 30 days before the date of the examination and closes 10 days before it. Candidates are informed of the location of the examination by email, four days in advance. Students who have not registered for an examination run the risk of being refused admittance to the examination, if space is not available.

Symbols used in the examination registration system:

\*\* denotes that the examination is being given for the penultimate time.

\* denotes that the examination is being given for the last time.

### **Code of conduct for students during examinations**

Details are given in a decision in the university's rule book:  
<http://styrdokument.liu.se/Regelsamling/VisaBeslut/622682>.

### **Retakes for higher grade**

Students at the Institute of Technology at LiU have the right to retake written examinations and computer-based examinations in an attempt to achieve a higher grade. This is valid for all examination components with code "TEN" and "DAT". The same right may not be exercised for other examination components, unless otherwise specified in the course syllabus.

### **Retakes of other forms of examination**

Regulations concerning retakes of other forms of examination than written examinations and computer-based examinations are given in the LiU regulations for examinations and examiners,

<http://stydokument.liu.se/Regelsamling/VisaBeslut/622678>.

### **Plagiarism**

For examinations that involve the writing of reports, in cases in which it can be assumed that the student has had access to other sources (such as during project work, writing essays, etc.), the material submitted must be prepared in accordance with principles for acceptable practice when referring to sources (references or quotations for which the source is specified) when the text, images, ideas, data, etc. of other people are used. It is also to be made clear whether the author has reused his or her own text, images, ideas, data, etc. from previous examinations.

A failure to specify such sources may be regarded as attempted deception during examination.

### **Attempts to cheat**

In the event of a suspected attempt by a student to cheat during an examination, or when study performance is to be assessed as specified in Chapter 10 of the Higher Education Ordinance, the examiner is to report this to the disciplinary board of the university. Possible consequences for the student are suspension from study and a formal warning. More information is available at <https://www.student.liu.se/studenttjanster/lagar-regler-rattigheter?l=sv>.

### **Grades**

The grades that are preferably to be used are Fail (U), Pass (3), Pass not without distinction (4) and Pass with distinction (5). Courses under the auspices of the faculty board of the Faculty of Science and Engineering (Institute of Technology) are to be given special attention in this regard.

1. Grades U, 3, 4, 5 are to be awarded for courses that have written examinations.
2. Grades Fail (U) and Pass (G) may be awarded for courses with a large degree of practical components such as laboratory work, project work and group work.

### **Examination components**

1. Grades U, 3, 4, 5 are to be awarded for written examinations (TEN).
2. Grades Fail (U) and Pass (G) are to be used for undergraduate projects and other independent work.

3. Examination components for which the grades Fail (U) and Pass (G) may be awarded are laboratory work (LAB), project work (PRA), preparatory written examination (KTR), oral examination (MUN), computer-based examination (DAT), home assignment (HEM), and assignment (UPG).
4. Students receive grades either Fail (U) or Pass (G) for other examination components in which the examination criteria are satisfied principally through active attendance such as other examination (ANN), tutorial group (BAS) or examination item (MOM).

The examination results for a student are reported at the relevant department.

### **Regulations (apply to LiU in its entirety)**

The university is a government agency whose operations are regulated by legislation and ordinances, which include the Higher Education Act and the Higher Education Ordinance. In addition to legislation and ordinances, operations are subject to several policy documents. The Linköping University rule book collects currently valid decisions of a regulatory nature taken by the university board, the vice-chancellor and faculty/department boards.

LiU's rule book for education at first-cycle and second-cycle levels is available at [http://stydokument.liu.se/Regelsamling/Innehall/Utbildning\\_pa\\_grund-\\_och\\_avancerad\\_niva](http://stydokument.liu.se/Regelsamling/Innehall/Utbildning_pa_grund-_och_avancerad_niva).