SK2820 Molecular Physics 8.0 credits

Molekylfysik

This is a translation of the Swedish, legally binding, course syllabus.

If the course is discontinued, students may request to be examined during the following two academic years

Establishment

Course syllabus for SK2820 valid from Autumn 2007

Grading scale

A, B, C, D, E, FX, F

Education cycle

Second cycle

Main field of study

Physics

Language of instruction

The language of instruction is specified in the course offering information in the course catalogue.

Intended learning outcomes

This course equips you with the tools to build yourself a “molecular toolkit” and provides you with the opportunities to use these to investigate, discuss and explore the physical basis of molecular properties. After the course, you will be able to:

- discuss the fundamental differences between atoms and molecules.
- show how the molecular bonds can be described theoretically by applying some fundamental approximations. The consequences of the approximations should be understood.
- discuss molecular bonding in terms of the molecular orbitals. Knowledge on the molecular system can be obtained by using Walsh diagrams (or correlation diagrams).
- determine the electronic state symmetry using the electron configuration. This demands some basic knowledge in group theory.
- to measure molecular properties such as molecular geometry (internuclear distances and angles), dipolemoments and polarizabilities and electronic state energies.
- set up simple models for the interaction between molecules.
- describe the fundamental approximations used in the most common quantum chemistry methods. Also you should be able to use the Gaussian program to obtain fundamental information on simple molecular systems.
- discuss what determines the geometry of a polyatomic molecule, by using the hybrid orbitals and the Hückel molecular orbital theory.

Course contents

The course consists of 18 scheduled lectures of 2 hours each. The course has been divided into 6 areas:

- Introduction and chemical concepts.
- Intramolecular bonding.
- Molecular structure and spectroscopy.
- Intermolecular interaction and bonding.
- Quantum chemistry.
- Elements of molecular dynamics and chemical reaction kinetics.

After each area, homework problems will be given. These problems will be of both experimental and theoretical nature or computer calculations.

Specific prerequisites

Course literature

N. H. March and J. F. Mucci, Chemical Physics of free molecules, Plenum Press (the edition used will be announced on the course homepage at least four weeks prior to start of the course).

Examination

- TEN1 - Examination, 8.0 credits, grading scale: A, B, C, D, E, FX, F

Based on recommendation from KTH's coordinator for disabilities, the examiner will decide how to adapt an examination for students with documented disability.

The examiner may apply another examination format when re-examining individual students.

Other requirements for final grade

The course is examined by an oral exam (TEN1, 8 hp, grading A/B/C/D/E/Fx/F). Approved home assignments and laboratory work is required to take the oral exam.

Ethical approach

- All members of a group are responsible for the group's work.
- In any assessment, every student shall honestly disclose any help received and sources used.
- In an oral assessment, every student shall be able to present and answer questions about the entire assignment and solution.