Syllabus

for course in education at postgraduate level Yt- och vätskefysik Surface and Liquid Physics

Course code: Valid from: Established: Department: FK40003 VT 2018 2017-12-14 Department of physics

Subject:

Chemical physics

Decision

Denna kursplan är fastställd av Fysikums styrelse 2017-12-14.

Prerequisites and special admittance requirements

Admitted to graduate level education

Course objectives

The course aims to broaden the doctoral student's research area: chemical physics

Content

The course covers: Introduction to symmetry concepts, structure and categorization of surfaces and surface adsorbates. Fundamental bonding and electronic structure of molecules on surfaces. Surface and catalytic reactions. Experimental techniques for measuring structure, electronic structure and dynamics on surface adsorbates and during catalytic reactions. Synchrotron light and X-ray laser experiments. Theoretical methods for describing chemical bonding and reactions on surfaces. Electrocatalytic processes with a focus on renewable energy production and energy conversions.

Thermodynamic and dynamic properties of simple liquids in particular water. Structure measurements based on X-ray and neutron measurements. Experimental methods of dynamics. Molecular dynamics simulations. Supercooled water, amorphous ice and glass state. Hypotheses around liquid transitions and critical point for water. Aqueous solutions with ions and biomolecules.

Learning outcome

After completing the course, the student is expected to:

- * be able to account for and apply symmetry classification of surface adsorbates
- * be able to assess the applicability of the various models for chemical bonding to and dynamics on surfaces
- * based on the d-band model, be able to predict the activity of various transition metals in selected reactions in heterogeneous catalysis

* describe the elementary reaction steps that determine the extra voltage that is lost or must be added during electrocatalytic processes

- * be able to account for the difference in properties of a normal liquid and water
- * describe different methods to obtain structure and dynamic information about liquids with a focus on water
- * be able to explain the principles of conducting molecular dynamics simulations with liquids

10 Högskolepoäng 10 ECTS credits * describe the phase diagram of water in terms of amorphous ice, glass state, supercooled water, critical point and liquid transitions

* be able to explain how aqueous solutions differ from pure water in terms of structure and dynamics

Forms of instruction

Instruction consists of lectures and seminars.

Participation in lectures and seminars is mandatory. If there are special reasons, the examiner can, after consultation with the relevant teacher, grant the student exemption from the obligation to participate in certain compulsory teaching.

The teaching takes place in English.

Forms of examination

The course is examined in the following way:

- a. knowledge is checked through a written test, assignments, oral reports and activity at seminars. Examination takes place in English.
- b. Grading according to a two-point grading scale: Pass or Fail.
- c. The course's grading criteria are distributed at the start of the course.

d. Students who fail the regular exam have the right to undergo additional exams as long as the course is given. The number of test occasions is not limited. With exams, other compulsory course parts are also included.

Transitional provisions

Students can request that the examination be carried out according to this syllabus even after it has ceased to apply, however, no more than three times during a two-year period after teaching on the course has ended. This should be requested to the institution's board. The provision also applies when revising the syllabus.

Restrictions

The course cannot be included in the degree together with the course FK7044 or the equivalent.

Course literature

Course literature is announced well in advance of the start of the course.