CHEMISTRY COURSES 2017-2018

KEMS320 Advanded Course in Inorganic Chemistry 1 - Main Group Chemistry 3ECTS

Advanced level, Master level
Teacher: Jari Konu

Study Objectives

After passing the course, the student will:

- have a basic understanding of main group chemistry,
- understand the connection between electronic structure and molecular properties,
- know the basics of inorganic characterization methods and their uses in research and industry,
- understand the basics of writing scientific manuscripts, and
- have gained experience in preparing and delivering scientific research presentations.

Course description

The course includes topics such as:

- main group chemistry (groups 1, 2 and 13 - 18),
- organometallic compounds of main group elements,
- MO- and VB-theories,
- total electron density and bonding, and
- characterization methods in inorganic chemistry.

Completion mode

Active participation in lectures, mandatory seminar presentation on a topical issue in main group chemistry based on review of articles in scientific journals, and passing the home exam at the end of the course.

On academic years when lectures are not given: taking the course is possible by completing home exam and giving seminar presentation (contact the lecturer for scheduling).

Prerequisites

Subject studies in chemistry, especially courses KEMA214 and KEMA215 (Inorganic Chemistry 1 and 2).

Evaluation criteria

Evaluation based on home exam at the aend of the course, 50% of the total points required to pass. In addition, seminar presentation is mandatory for the completion of the course.

KEMS321 Advanded Course in Inorganic Chemistry 2 - Organometallic Chemist 3 ECTS
Advanced level, Master level
Teacher: Matti Haukka

Study Objectives

Understanding the structures and reactions of the most common organometallic compounds.

Course description

- Introduction to organometallic chemistry
- General properties of organometallic compounds
- Typical organometallic compounds and reactions
- Homogeneous catalysis
- Applications of organometallic chemistry

Completion mode

Final exam

Evaluation criteria

To pass the course with grade 1, at least 50% of the available points on the final exam must be achieved.

KEMS3800 Advanced laboratory exercises of inorganic structural and synthetic chemistry 1-12 ECTS

Teacher: Manu Lahtinen
Fall Term

Study Objectives
After successfully completing the course, the student:

- is familiar with safe laboratory working practices, different structural and synthetic chemistry oriented methods, as well as with common extraction, purification and characterization techniques.
- Understands the applicability of various structural chemistry oriented characterization techniques, and has some basic knowledge on how to utilize them.
- Understands the theoretical basis of the most common methods in structural chemistry and knows how to apply them to resolve simple analytical problems.
- Knows how to handle air - and moisture sensitive materials, and can apply the techniques to perform simple air- and moisture sensitive synthesis.
- Has basic knowledge on routine molecular modelling programs and methods, and can perform simple modelling tasks.

Course description

Advanced Inorganic and Analytical Chemistry Laboratory Work focuses on synthetic inorganic chemistry as well as different characterization methods and instruments used in chemical analysis. The course consists of pick-and-choose modules that typically concentrate on one particular technique like the handling of air and moisture sensitive compounds, molecular modelling, X-ray diffraction, thermogravimetry and different spectroscopic methods such as atomic absorption and emission spectroscopy. Students can register for all modules (except mini project work) through Korppi's teaching groups after which further information about the module (pre-assignments, supervision and scheduling) can be obtained from its instructor. Registrations must be made well in advance to allow sufficient time for all practical arrangements.

Module subjects and ECTS credits:

1.Single crystal structure determination (starting from a pre-measured dataset), 2 ECTS credits

- prerequisite for the module is successful pass of the Principals of X-ray diffraction methods KEMS3250

2. Preparation and characterization of paramagnetic materials, 2 ECTS credits

3. Characterization of solid materials with X-ray radiation based methods, 1 + 1 ECTS credits
- Module can be made in 1 or 2 credits

4. Synthesis and characterization of ionic liquids and their precursor salts, 2 ECTS credits

5. Molecular modelling, 1 + 1 ECTS credits
- module can be made in 1 or 2 credits

6. Handling of air and moisture sensitive compounds, 2 ECTS credits

7. Mini project, 2 - 6 ECTS credits *

* Mini projects offer a possibility to work in a research group for a short period of time and conduct independent, yet supervised, research on a given topic. ECTS credits earned depend on the duration of the mini project. For example, full-time work (35 h/week) in the laboratory for one month is equivalent to 5 ECTS credits. Students can do either one or several mini projects and can also split their working time among different research groups. Further details about mini projects can be obtained from research group leaders (Matti Haukka, Jari Konu, Manu Lahtinen ja Heikki Tuononen).

Completion mode

In addition to the practical laboratory work, the completion of each module requires a written laboratory report and/or presenting results in a research seminar. Laboratory reports (written by each student) will be read by the instructor who also marks the reports and gives feedback (graded passed-failed). Seminar presentations (15 minutes) take place at research group meetings and are not evaluated. However, each presenter receives individual feedback from the participants.

Registration:

Students can register for all modules (except mini project) through Korppi's teaching groups after which further information about the module (pre-assignments, supervision and scheduling) can be obtained from its instructor during the start date of the module.

Workload:

Most modules can be completed within one to two weeks' time. The working hours for each day vary considerably, which generally allows active participation at lectures concomitantly with the laboratory work.

The ECTS credits listed for each module include not only the time spent in the laboratory but also the time used for pre-assignments (reading laboratory manuals, searching for relevant literature and project planning) as well as for writing laboratory reports and/or preparing and presenting seminar talks.

Prerequisites

Subject studies in chemistry, in particular KEMA214, KEMA215, KEMA220 and KEMA250.

Evaluation criteria

For each module credits: successful passing of experimental work and corresponding report.

KEMS541 Advanced Course in Organic Chemistry, 6 ECTS
Teacher: Petri Pihko
Fall term

Study Objectives

The goal of the course is to lay foundations for synthetic, structural and strategic thinking in organic chemistry based on structure-reactivity relationships.

Course description

Nucleophiles and electrophiles, carbonyl chemistry (revision), conformational analysis, nucleophilic and electrophilic reactivity in saturated and unsaturated systems, prediction of selectivity, enolate chemistry and conjugate additions, radical chemistry, pericyclic reactions, transition metal-catalyzed reactions in e.g. coupling reactions.

Completion mode

Five problem sets (40% of the overall score) and two exams (one midterm, one final exam). Alternatively, a final exam.

Evaluation criteria

Problem sets, e-problems and the exam will be graded and the grade will be based on the total score acquired. Alternatively, the grade can be based on an exam alone.

The problems and the exam will evaluate the students' ability to understand functional group reactivity, structural effects on reactivity and conformational analysis, mechanistic thinking, and reaction mechanisms.

KEMS5800 Advanced practical laboratory of organic structural and synthetic chemistry, 1-12 ECTS
Teacher: Tanja Lahtinen

Spring and Fall term

Study Objectives

After the course the student knows the basic analytical techniques in organic synthesis and structural chemistry. The aim of the course is to give information how to use different analytical methods. The student is able to use different analytical methods in the structural elucidation of an unknown compound. Student knows how to use modern synthesis procedures. The student will learn how to use advanced laboratory techniques and handling. The student is able to carry out modern organic synthesis with confidence and in such a way as to maximize the chance of success. In mini project work student learn how to work in research group and to get the insight of the research fields in organic synthesis and structural chemistry, in the University of Jyväskylä.

Course description

Practical advanced laboratory works includes introduction lecture before starting the practical laboratory works. This will be organized in mid-September.

Advanced practical laboratory work in organic synthesis and structural chemistry consist of synthesis and analytical work of organic chemistry and instrumental analysis, multi-phased synthesis with laboratory book keeping on the progress of the synthesis. Project work, is done mainly in research groups, before Master project.

Completion mode

For more information please contact University lecturer Tanja Lahtinen

Prerequisites

Students who have organic chemistry as a major should have Organic Chemistry (KEMA282/283) Organic Chemistry Laboratory work (KEMA239) and KEMA250 completed.

Evaluation criteria

Successful passing of experimental work and corresponding report.

KEMS3250 Principles of X-ray diffraction methods, 6 ECTS

Teachers: Kari Rissanen, Manu Lahtinen
Spring term every year

Study Objectives

After successfully completing the course, the student:

- understands basic principles of X-ray crystallography, and knows in the basic level how to apply them for characterizing crystalline materials with single crystal diffraction method.
- Understands common practices in X-ray diffractometry and is aware of sample and instrumentation related parameters effecting to analysis.

Course description

Course focuses on:

- X-ray radiation, crystal systems, Bravais lattices, symmetry operations and space group symmetries,
- measurement techniques, structure determination procedures, depicting methods and programs
- Course includes instrument demonstration and structure determination exercise

Completion mode

Exercises, instrument demonstration, and final exam at the end of the course

Prerequisites

Subject studies in chemistry

Evaluation criteria

Exercise and final exam at the end of the course, or book exam.

KEMS526 Modern Synthetic Organic Chemistry 6 ECTS
Teacher: Petri Pihko

Spring Term

Study Objectives

The goal of the course is to boost the skills of students in the use of modern synthetic methods in the planning of organic syntheses and to provide key tools for critical evaluation of synthetic strategies. The purpose of the seminar is to provide the students an opportunity to draft proposals for synthetic routes in small groups and to learn to evaluate and criticize the synthesis plans in a seminar setting.

Course description

Organic reactivity, C=C- and C-C coupling methods, stereochemical strategies, cyclic and acyclic diastereoselectivity, advanced strategies, key methods of asymmetric and stereoselective synthesis. The course consists of a two-stage seminar that includes planning of a synthetic strategy as well as five home exercises. There is no final exam.

Completion mode

Five problem sets (totaling 50% of the overall score) and a two-stage seminar where the students present a synthesis plan for their chosen target molecule.

Evaluation criteria

The problem sets are graded with a score of 0-10 for each problem.

The synthesis plan of the seminar presentation (only the final version) will be graded using the following criteria:

- the credibility and feasibility of the plan. Are there clearly erroneous steps, or steps which are not clearly justified? (20 p)

- the shortness and originality of the plan. (20 p)

- presentational points. Are the literature citations proper and correct? Are the presentation slides clear? Is the presentation logical? (10 p)

The seminars are public and the grading is also based on the collective evaluation based on collected feedback during the presentation.

Please note that your personal style of presentation is not going to be judged.

KEMS532 Supremolecular Chemistry, 6 ECTS

Teacher Maija Nissinen

Book Exam and Independent home work on Year on year 2017-2018

Study Objectives

The student knows basic concepts and phenomena of supramolecular chemistry and recognizes the most typical supramolecular compounds. The student understands the role of the weak interactions and can design simple supramolecular receptor molecules. The student knows basic concepts, research methods, interactions and applications of solid state supramolecular chemistry. The student understands the concept and the most typical applications of self-assembly. The student can design simple potential supramolecular machines and biomimetic models.

Course description

Basic concepts of supramolecular chemistry: weak interactions, cooperativity, complementarity, preorganization, template effect, self-assembly, complexation. Cation, anion and ion pair receptors: crown ethers, podands, cyclodextrins, calixarenes and cyclophanes. Molecular machines and devices. Supramolecular chemistry of life and biomimetic structures.

Completion mode

The course can be taken either by learning exercises or book exam 2017-2018

Prerequisites

Subject studies in chemistry or bachelor level studies for nanoscience students.

Evaluation criteria

The course grading is based on course activity and learning outcomes achieved or the results of the exam. Grade 1 equals for 50 % of maximum points.

KEMS531 Introduction to material Chemistry 4 ECTS

Teacher Maija Nissinen

Fall Term

Study Objectives

The student knows basic concepts, synthetic methods, properties and applications of polymers and hybrid materials.

Course description

The course concentrates on basic concepts of organic and nanomaterial chemistry. Basics of polymer chemistry. Gels, liquid crystals, self-assembling monolayers and surfaces. Introduction to concepts of material chemistry: composites, nanocomposites, nanoparticles, hybrid and functional materials, porous materials, biomaterials. Material synthesis, characterization and applications in medicine, optics, electrical chemistry, molecular electronics and coatings.

Completion mode

Learning exercises, independent and pair work during the course; learning exercises.

Prerequisites

Subject studies in chemistry or bachelor level studies for nanoscience students.

Evaluation criteria

The course grading is based on course activity and learning outcomes achieved. Grade 1 equals for 50 % of maximum points.

KEMS534 Basic Principles of Mass Spectrometry, 4 ECTS

Study Objectives

After the course, student understands the basic concepts of mass spectrometry and essential operational principles of most general ion sources and mass analyzers. A student is able to choose a suitable mass spectrometric method for an analytical problem and to predict and interpret simple mass spectra obtained by different methods.

Course description

Course concentrates on basic concepts of mass spectrometry, interpretation of mass spectra as well as on structures and operational principles of different mass spectrometers. In addition basics of tandem mass spectrometry and most general applications of mass spectrometry will be discussed. Lectures will be held in english if one of participants is english speaking.

Completion mode

Completion 1, as a course: completion consists of exercisises, exam and laboratorio visit. Student must then obtain at least 1/3 from maximum points of exercises, 1/3 maximum points in exam and at least 50% of the combined points.

Completion 1, as book exam: student must obtain at least 50 % from the maximum points in exam.

Evaluation criteria

Completion 1: participation in exercises (at least 33.3%), participation in exam, participation in laboratory visit

Completion 2: participation in exam

KEMS5380 Basics of NMR Spectroscopy, 4 ECTS
Teacher Elina Sievänen

Study Objectives

The student knows the basic terms and phenomena related to NMR spectroscopy, and familiarizes him/herself to the instrumental considerations, data collection, and processing at a theoretical level. The student understands how the information obtained by NMR spectroscopy can be used in determining the structures of unknown compounds, and is able to analyze simple NMR spectra. Moreover, the student is aware of the most common NMR experiments and is able to use them for practical purposes.

Course description

The aim of this course is to explore nuclear magnetic resonance as a phenomenon and to cover factors influencing on chemical shifts and spin-spin coupling (first and higher order couplings) together with 1D/2D NMR experiments based on it in more detail. Within the exercises simple 1D/2D NMR spectra will be analyzed. Additionally, instrumental considerations, data collection, and processing are introduced at a theoretical level.

Completion mode

Lectures, exercises, and exam
Book exam

Prerequisites

Basics of NMR Spectroscopy

Evaluation criteria
Exam: 4 x 6 p = 24 p

By returning written exercises the student may earn 3 x 2 p = 6 p

Grading:

> 23 p = 5

20-22 p = 4

17-19 p = 3

14-16 p = 2

11-13 p = 1

< 11 p = F

KEMS5390 Käytännön NMR-spektroskopia, 2 ECTS
Teacher Elina Sievänen

Study Objectives

After completing the course the student is able to utilize 1D and 2D NMR spectroscopy in solving the structures of unknown compounds in the forms of spectral interpretation and the use of the Bruker FT NMR spectrometer(s) of the Department of Chemistry.

Course description

1H-, 13C-, 13C DEPT-135-, 1H-1H COSY-, 1H-13C HMQC- and 1H-13C HMBC NMR-spectra and their utilization in structural analysis, sample preparation, measurement of spectra and processing of the data, spectral interpretation exercises, and demonstration on the spectrometer.

Completion mode

In order to complete the course the student has to perform the necessary NMR measurements for solving the structure of an unknown compound and to give a written report of its structural analysis.

Prerequisites

Basics of NMR Spectroscopy

Evaluation criteria

In order to complete the course the student has to perform the necessary NMR measurements for solving the structure of an unknown compound and to give a written report of its structural analysis. The structure of the compound has to be correctly analyzed for passing the course.

KEMS544 Macromolecular NMR spectroscopy 3-5 ECTS
Teacher Perttu Permi

Study Objectives

The course is divided in two parts, introductory level (3 ECTS) and advanced level (2 ECTS). In the introductory level course, the student will learn basics of multinuclear multidimensional NMR spectroscopy and how NMR spectroscopy can be applied to study structure and function of biological macromolecules, mainly proteins. Student will learn and understand different steps involved in protein structure determination; sample preparation, data collection using various NMR experiments, data processing, data analysis, structure calculations and validation of structures. In addition, student will learn how to utilise NMR spectroscopy to study protein dynamics and molecular interactions.

In the advanced level course (2 ECTS), the student obtains more profound level knowledge of various NMR experiments. He/she understands on theoretical and practical level how different NMR experiments work, how they can be analyzed and how to modify the existing experiments and design new ones.

Course description

The course will cover how to study structure and function of biological macromolecules, mainly proteins, by multidimensional multinuclear NMR spectroscopy.

The course has been divided in two parts, introduction level (3 ECTS) and advanced level (2 ECTS) course. The student can participate either introduction level course or both courses at the same time (courses are run parallel). However, in order to receive 5 ECTS, participation for both courses is required, that is, there is no possibility to participate advanced level course without completing the introductory level course.

Completion mode

Three final exams will be organised. Questions in the final exam cover the topics in lecture material, topics discussed during the lectures and practical sessions. In addition, students need to accomplish/pass one or several assignments given out during the course. These can be done either individually or working in small groups.

Prerequisites

Prior passing or simultaneous participation to introductory level course (3 ECTS) is mandatory in order to participate advanced level course (2 ECTS).

Participation and passing of courses KEMS5380 Basics of NMR Spectroscopy (4 ECTS) ja KEMS5390 Practical NMR Spectroscopy (2 ECTS) is not required but highly recommended.

Evaluation criteria

The course grading uses the numerical scale from 1 to 5. In order to pass the course, student must pass/accomplish the assignment given out in lectures/practices. In addition, student needs minimum of 50% of maximum points available from the final exam (3 ECTS introductory level course). Passing of advanced level course necessitates passing of introductory level course (3 ECTS) with aforementioned criteria and obtaining > 50 % of maximum points of advanced level course final exam.

Thus, student may obtain either 3 or 5 ECTS, but the grading is based on performance on introductory level course exam (1-5).

KEMS401 Quantum Chemistry 6 credits
Teacher Karoliina Honkala
Fall Term

Study Objectives

A student, who has passed the course, has deepened his/her understanding of the theory of quantum mechanics. He/she is familiar with Dirac's bra and ket formalism and can apply it to a harmonic oscillator. In addition, the student is able to solve simple quantum mechanical problems using wave mechanics both exactly and with different approximation methods. She/he knows how to apply perturbation theory to describe the interaction of atoms and molecules with electromagnetic radiation, and understands the origin of covalent bond.

Course description

The Fundamentals of quantum mechanics including, operators, eigenvalue equations, commutators, the Schrödinger equation, particle in a box model, harmonic oscillator, hydrogen atom, time-independent and time-dependent perturbation theory, variational theorem, absorption and emission of electromagnetic radiation, and the covalent bond.

Completion mode

The course will be lectures in English if needed. Lectures willl take place in the first period of the fall semester every year. To complete the lecture course a student will take two class tests. At another time, a student can pass the course by taking a final exam.

Prerequisites

Physical chemistry 2 course (KEMA225)

Evaluation criteria

The course can be completed either with two class tests (during lectures) or by taking one final exam.

For class tests, a student can earn extra points by solving actively demo problems.

KEMS4150 Optical Spectroscopy 3-6 credits
Teacher Mika Pettersson
Fall term

Study Objectives

The study module can be taken at two levels with different objectives: basic level corresponding to 3 credit points and advanced level corresponding to 6 credit points.

At the basic level, student understands the basics of the interaction between electromagnetic radiation and matter and additionally the basics of experimental spectroscopic methods. Student understands the principles of vibrational, electronic and photoelectron spectroscopy and can interpret spectra related to these spectroscopies. Student understands basic principles of lasers and laser spectroscopy and photochemical and photophysical processes.

At the advanced level, in addition to the objectives of the basic level, student reaches deeper theoretical understanding of the topics. Additionally, student understands the basic theory of energy transfer, electron transfer, light scattering and femtosecond spectroscopy and the main experimental methods in femtosecond spectroscopy. Additionally, student understands basic theory of spectroscopy of metallic and plasmonic systems, semiconductors, and solid state matter.

Course description

Interaction between electromagnetic radiation and molecules, experimental methods, vibrational spectroscopy, electronic spectroscopy, photoelectron spectroscopy, laser spectroscopy photochemical and photophysical processes.

Completion mode

Study module can be passed by participating the lecture course or by taking a final exam. The lecture course contains lectures and exercises. Part of the exercises (1/3) are obligatory and the additional exercises will give extra points. There is one exam at the lecture course.

Prerequisites

Basic level: KEMA225 (physical chemistry 2) or equivalent.

Advanced level: KEMS412 (symmetry and group theory in chemistry) or equivalent, and KEMS401 (quantum chemistry) or equivalent. KEMS401 can also be taken simultaneously.

Evaluation criteria

Test: max 18 p
exercises: max 4 p.

KEMS4800 Optical Spectroscopy Laboratory, 1-12 ECTS
Teacher Toni Kiljunen

Study Objectives

Students acquire profound understanding and mastery of experimental phenomena and theoretical concepts in physical chemistry. They learn principles of current research topics in optical spectroscopy, and become capable of analyzing the results. Students familiarize themselves with experimental setups and measurement techniques in laser laboratory. Students can work independently in the laboratory and are able to write comprehensive measurement reports. They can consider the reliability of the measurements and show how the results relate to literature values.

Course description

The course consists of four branches: (A) Analytical spectroscopy, (B) Structural spectroscopy, (C) Applied photochemistry, and (D) Photochemistry research. In A, qualitative analysis is performed for a natural sample, for a pharmaceutical sample, or for a sample mixture. In B, structural parameters are obtained for small molecules in gaseous or liquid phase. In C, photoreactions and laser device techniques are studied. In D, time-dependent phenomena are investigated.

Completion mode

Independent work in the student laboratory, and small-group work in the laser laboratory. Written reports on the assignments, each 1-2 ECTS worth. Starting session is organized for choosing the assignments and arranging the schedule.

Prerequisites

Bachelor level physical chemistry courses or equivalent studies. Knowledge of optical spectroscopy, molecular symmetry and group theory in chemistry (KEMS4150 and KEMS412 or equivalent) is recommended.

Evaluation criteria
Scientifically sound reports on assignments.

KEMS4180 Chemical dynamics and molecular interactions 3-6 ECTS
Teacher Gerrit Groenhof

Study Objectives

The aim of the course is to unify the concepts from previous quantum chemistry courses (molecular structure, molecular interactions) and thermodynamics courses (material properties, reaction rates). The students will become familiar with the basic concepts of statistical thermodynamics and can apply them to chemical problems. Student will understand how intermolecular interactions are related to macroscopic properties and how the latter can be obtained from first principles.

Course description

Statistical mechanics, energy, entropy, ensembles, partition functions, free energy, molecular interactions, transition state theories.

Completion mode

Written exam

Prerequisites

KEMA224 Physical Chemistry 1
KEMA225 Physical Chemistry 2

Evaluation criteria

The written exam will evaluate the students' understanding of the course material and his or her ability to compute macroscopic thermodynamic quantities from microscopic properties.

A linear
Properties of matter based on

Ability to employ the concepts of statistical mechanics to compute properties of matter

KEMS409 Material Modelling 5 credits
Teacher Karoliina Honkala

Study Objectives

A student, who has passed the course, knows the basics of density functional theory and how to apply it to calculate simple chemical properties. She/he also knows the strong and weak points of the method. In addition, a student is familiar with different computational electronic structure analysis methods, can apply them into a simple systems and estimate possible errors. She/he will also be familiar with basics of molecular dynamic simulations

Course description

Introduction to density functional theory, the application of density functional theory to determine physical and chemical properties of materials, how to apply density functional theory to model various experimental parameters, time dependent density functional theory, calculation of activation energy for an elementary reaction step, atomistic thermodynamics, and introduction of molecular dynamics.

Completion mode

The course will be lectured in English if needed. Lectures will take place in the second period of the spring semester on even-numbered years. To complete the course, a student will carry out a computational project work and write an article-type of report of the obtained results. In addition to lectures, the course includes computational exercises.

Prerequisites

Basics of quantum mechanics. A student can discuss with the lecturer if his/her background is suitable to the class.

Evaluation criteria

A student's presence is obligatory in lectures and demo sessions. The evaluation of the class is based on the project work and the article-type written report of that work.

KEMS412 Symmetry and Group Theory in Chemistry 2 ECTS
Teacher Mika Pettersson
Fall term

Study Objectives

Student knows how to use symmetry operations and how to classify molecules into point groups. Student can apply group theory to vibrational spectroscopy and can determine the symmetry selection rules for infrared and Raman spectroscopy. Student understands how group theory is used in description of chemical bond and electronic spectroscopy.

Course description

Molecular symmetry, point groups, reducible and irreducible representations, projection operator, applications of group theory to vibrational spectroscopy, molecular orbital theory and electronic spectroscopy.

Completion mode

Study module can be passed by participating the lecture course or by taking a final exam. The lecture course contains lectures and exercises. Part of the exercises (1/3) are obligatory and the additional exercises will give extra points. There is final exam at the lecture course.

Prerequisites

Basic knowledge in chemistry. Basic knowledge in linear algebra is desirable but not obligatory

Evaluation criteria

Exam: max 18 p

exercises: max 3 p

9 points is required for passing.

KEMS4170 Fundamentals of electronic structure theory 5 ECTS

Teacher Gerrit Groenhof

Study Objectives

The course aims at providing the student with a detailed understanding of modern quantum chemistry methods and the necessary skills to apply these methods in a meaningful way to chemical problems.

Course description

Mathematical foundations of quantum chemical methods, Hartree Fock Theory, Perturbation Theory, Configuration Interaction, Density functional theory, semi empirical methods (MNDO, AM1, PM3), Quantum Monte Carlo.

In addition practical skills in performing calculations will be trained in two tutorial sessions.

Completion mode

The students will carry out a one-to-two week Computational Chemistry project in which he or she will apply quantum chemistry methods to reproduce results from older literature and validate those findings with more advanced calculations that possible on today's computer hardware.

The student will write a report about this project, in which also the methods are discussed and motivated.

Prerequisites

KEMS412 Symmetry and Group Theory in Chemistry, or equivalent

KEMS401 Quantum Chemistry (can be completed simultaneously), or equivalent

Evaluation criteria

To pass the course, the students need to demonstrate in the report and discussion that he or she understands the basic concepts and can motivate the choice of the method used in the project.

KEMS6800 Advanced laboratory exercises in renewable natural resources and chemistry of living environment, 1-12 ECTS

Teachers Ari Väisänen, Hannu Pakkanen, Jarmo Louhelainen

Study Objectives

Students familiarize themselves in practice with the chemistry, processing, and analytics of biomass or the chemical analytics of living environment.

Students can independently do particular sample treatment procedures and they can independently measure samples with chromatographic or spectroscopic equipment.

Students understand essentially the chemical reactions relating to the sample treatment procedures.

Students can fluently report their experimental work and the results of the study.

Course description

Individual, one-by-one suited laboratory exercises consisting of biomass processing and chromatographic/spectroscopic analyses together with different sample treatment techniques for above-mentioned measurements. Dissolution of sample using different sample pre-treatment methods. Soil and water analysis.

Completion mode

Completed laboratory exercises and accepted work reports.

Prerequisites

Intermediate studies in chemistry

Evaluation criteria

Completed laboratory exercises and accepted work reports.

NANS1001 Fundamentals in Nanoscience, 6 ECTS
Teacher Janne Ihalainen

Study Objectives

After passing this course the student have an overview about nanoscience. He/she recognizes the size-classes and the main properties of nano-objects. He/she can fundamentals of the theoretical and experimental techniques in nanoscience. After the course, he/she has a clear picture about scientific literature in nanoscience and he/she can fluently provide short concise presentations from various themes in nanoscience

Course description

The course is taught by specialists from fields of physics, chemistry and biology. Fundamentals of nanoscience. Introduction of the general ideas and concepts of nanoscience. Topics include physical, chemical and biological aspects of nanoscience and nanotechnology.

Completion mode

Every week includes 2-3 h lectures plus one optional hour for discussion. The course contains teamwork sessions, where students presents their findings on given topics in teams. Students also write essays about given topics about nano science. An estimated time for the home work is 8 h weekly. An exam takes place at the end of the course.

Prerequisites

Basic knowledge from physics, chemistry and biology.

Evaluation criteria

Accepted grade requires the basic knowledge from the nano sciences.The essays and team-works for each student will be evaluated individually. The weight of the exam is 50% of the whole grade

NANS1002 Seminar in Nanoscience 1, 3 ECTS
Teachers Andreas Johansson, Janne Ihalainen

Study Objectives

After the course the student has a comprehension about utilisation nano science in academia and society. He/She is understands the scientific integrity and is capable to utilise his/her knowhow in natural sciences pervasive. He/She can present scientific material in clear and condensed way both effective and pithily.

Course description

The course consists of conversational learning events, home works and oral presentations.

Completion mode

Attendance to the learning events, written material and oral talks.

Prerequisites

Bachelor in nanosciences or similar studies.

Evaluation criteria

Attendance in the learning events and seminars.

NANS1003 Practical course in nanoscience, imaging, 4 ECTS
Teachers Andreas Johansson, Janne Ihalainen

Study Objectives

After passing this course the student recognizes the size-classes of nano-objects and the basic principles of major imaging techniques. He/she knows the pros and cons of each used technique. After the course the student is also able to provide simple nano-particles and choose the most optimal imaging technique for his/her purposes. After the course the student can interpret the obtained results and is able to report the results in a clear manner.

Course description

In this course various imaging techniques in different disciplines in the nanosciences are introduced. The aim is to understand the basic principles of each technique and their benefits and drawbacks. The lab work will be done in the groups and with the imaging devices for scientific purposes in NSC. At the end of the course, there is a small seminar where all the basic principles of the techniques will be rehashed and the results will be compared.

Completion mode

Attendance to the lectures and lab work. Report from each of the work and a small talk in the final-seminar.

Prerequisites

Some laboratory experience is required for the course.

Evaluation criteria

Active participation for the labor work, clear and competent reporting manner. Good data handling skills.

NANS1004 Computational nanosciences 2 ECTS
Spring Term

Study Objectives

At the end of this course, students are able to relate computational research to experimental and purely theoretical research. Students can differentiate and classify different methods in computational nanoscience with respect to their central approximations, quantum-mechanical characters, and computational efficiencies. They are able to justifiably choose the most appropriate computational methods once given the material system and the properties under investigation as well as independently deepen their methodological knowledge whenever necessary.

Course description

Viewpoints to computational research (material systems, methods, analysis, processes, computational infrastructure); overview of various computational methods (many-body methods, density-functional theory, tight-binding model, classical force fields, discretized continuum); suitability of different methods to investigate nanomaterial properties; computational research at NanoScience Center.

Completion mode

Discussions and interactive events, research project, participants teach.

Evaluation criteria

Compulsory lecture attendance (one absence allowed, second absence requires extra work).
Assessment is based on project (written and oral presentation) and activity on lectures.