UNIVERSITY OF GOTHENBURG

DEPARTMENT OF CHEMISTRY AND MOLECULAR BIOLOGY

BROAD EDUCATION IN PHYSICAL CHEMISTRY OUR RESPONSE TO THE UKÄ COMMITTEE/PHYS CHEM, GU

INTRODUCTION

Physical chemistry is a broad field of study that combines principles from physics and chemistry to understand and explain the fundamental behavior of matter at the molecular and atomic level. It is an interdisciplinary area of science that deals with the study of chemical systems, their properties, and how they change with time, space, and energy. At the Department of Chemistry and Molecular Biology at the University of Gothenburg, the supervisors, examiners, and PhD students devoted to physical chemistry are spread over almost all research divisions, i.e., Analytical-, inorganic- and physical chemistry division, Organic and medicinal chemistry division, Biochemistry and structural biology division, and Atmospheric science division. The strength of this setting is the interdisciplinarity of the subject of studies; however, the challenge has been to coordinate a coherent curriculum for the PhD students in the topic. It is obvious that this has been seen as a weakness as based on the UKÄ evaluation. Based on the feedback from UKÄ, the Department has taken measures to ensure that the physical chemistry students will receive the broad and in-depth research education as expected.

ANALYSIS AND EXPECTATIONS

A curriculum for PhD students in Physical Chemistry should cover a diverse range of subjects that reflect the interdisciplinary nature of the field. Specifically, it should include a strong foundation in the fundamental principles of chemistry and physics, including courses on thermodynamics, quantum mechanics, statistical mechanics, and spectroscopy, and also provide a survey of current research in the field.

ACTION PLAN and FUTURE COURSES

1) To ensure that the PhD studies in Physical chemistry at the Department becomes more coherent, we will ***implement an examiner/supervisor committee*** that will meet twice a year and follow up the PhD students and the Physical chemistry curriculum and ensure that it provides the required breadth. Initially these meetings will be hosted and chaired by the Head of Department, being Professor in Physical Chemistry. Long term, one of the Examiners will be elected to take on this duty.

2) Establish the three Masters courses (i.e. KEM131, KEM170 and KEM552) given yearly as PhD level courses, with modified entry requirements and learning objectives suitable for PhD level. Each course leader is responsible for updating the course requirements for including PhD level well in time before upcoming course starts. These core courses will help students develop a solid understanding of the principles governing chemical and physical behavior, which they will need to apply to solve complex problems and carry out original research in the field. A comprehensive curriculum that includes a strong foundation in fundamental principles, as well as specialized training in advanced

topics, and an emphasis on interdisciplinary research and communication skills is essential for PhD students in Physical Chemistry to become successful researchers in this exciting field.

3) Implement the new PhD-course NFKE309 Molecular quantum mechanics - a seminar series, 7.5 hp, to be given at a biannual rate. This new course is expected to be given in first time in starting in Jan 2024. This new course will be strongly recommended to all our PhD students in Physical Chemistry, and will ensure that all will be given a broad and deep understanding of the fundamentals of quantum mechanics, a central topic in Physical chemistry, independently of specific research field.

The Syllabi for the courses are attached. Note that the Department are moving to the new premises of Natrium in Aug-Sept 2023. This means that all physical chemistry teachers as well as students will be gathered in the same building. This is expected to benefit the PhD education in physical chemistry, and stimulate the interactions to provide the broad and in-depth knowledge in the field.

CONCLUSIONS

By the above action plan for updated curriculum for PhD-level education in Physical Chemistry, we intend to substantially strengthen the course syllabi for our PhD students, and use our resources wisely in order to provide a range of courses to guarantee for a broad education in physical chemistry, complementing the specialized expertise that they develop from their thesis work. The action plan, has numerous merits. Firstly, it contributes to that students receive a cutting-edge education that is relevant to current research in the field, specifically focusing on the new course NFKE309 Molecular quantum mechanics 7.5 hp. Secondly, bringing together students from the different groups into a common seminar-based course, combined with moving together in Natrium, creates a sense of community and collaboration between students and faculty within the department, leading to enhanced networking and research opportunities. Thirdly, this internal course program provides flexibility and customization of the curriculum to meet individual student needs, at the same time as it complements the specific research topic of a student to achieve a broad and in-depth education in physical chemistry.

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DEPARTMENT OF CHEMISTRY AND MOLECULAR BIOLOGY

NFKE309 Molecular quantum mechanics - a seminar series, 7.5 credits

Molekylär kvantmekanik - en seminarieserie, 7,5 högskolepoäng

Third-cycle level / Forskarnivå

Confirmation

This syllabus was confirmed by the Department of Chemistry and Molecular Biology on 2023-04-06, and is valid from Autumn semester 2024.

Responsible Department
Department of Chemistry and Molecular Biology, Faculty of Science

Entry requirements

To be admitted to the course, students must have:

- Passed the general entry requirements for higher education in Natural Science specializing in Chemistry, Biophysics or similar.
- have passed 90 HEC in science courses, comprising at least:
  - General Chemistry 15 HEC
  - Inorganic Chemistry- Basic Course 7.5 HEC
  - Organic Chemistry- Basic Course 7.5 HEC
  - Physical Chemistry- Basic Course 15 HEC or 7.5 HEC combined with 7.5 HEC Basic physics
  - Mathematics for Scientists 15 HEC
- or at least 30 HEC in mathematics combined with 75 HEC in physics including:
  - Atomic and Molecular Physics 7.5 HEC
  - Solid State Physics 7.5 HEC
- requirements for English proficiency corresponding to at least level B2

Learning outcomes

Knowledge and understanding

Upon completion of the course the student shall

- demonstrate broad knowledge and systematic understanding of Molecular Quantum Mechanics, focusing on

    - The foundations of QM such as the wave function, operators, postulates and evolution of states.
    - Linear and rotational motion, the harmonic oscillator and Angular momentum
    - The hydrogen atom and atomic spectra
    - The Born-Oppenheimer approximation and molecular orbital theory
    - Spectroscopy based on rotational, vibrational, and electronic transitions.
- demonstrate familiarity with approximation methods and introduction to group theory.

Competence and skills

Upon completion of the course the student shall

- demonstrate the capacity to review and perform a lecture on a selected course topic autonomously
- demonstrate the ability to reflect upon and critically analyze QM concepts and theories, and discuss these with fellow students.
- Analyze and solve QM exercises and problems using appropriate methods

Judgement and approach

Upon completion of the course the student shall

- critically reflect on the possibilities and limitations of QM, in the context of the research project of the student as well as in relation to its role in society
- be able to speculate about future development and direction of QM, particularly in view of computational technologies and sustainable development.

Sustainability labelling

The course is sustainability-related, which means that at least one of the learning outcomes clearly shows that the course content meets at least one of University of Gothenburg's stipulated criteria for sustainability labelling.

Course content

Quantum mechanics (QM) account for the behavior of atoms and molecules at the most fundamental level. Thereby, QM is a central subject in order to understand the properties of all matter, ranging from technologically advanced materials to the processes taking place within living organisms. In this course, the theoretical concepts of QM are brought into focus in form of a seminar series, by which the doctoral students themselves take the lead in dwelling into the contents.

The course covers the following topics

- The foundation of QM
    - The characteristics of wavefunctions
    - Operators, postulates and evolution of states
- Linear and rotational motion
    - Particle in a box, on a ring, and on a sphere
    - The harmonic oscillator
    - Motion in a Coloumbic field
    - Angular momentum

- The spectrum of hydrogen, helium and many-electron atoms
- An introduction to molecular structure
    - Born-Oppenheimer approximation
    - Molecular orbital theory
    - The band theory of solids
- Spectroscopic transitions including
    - Absorption, emission and Raman processes
    - Rotational, vibrational, and electronic transitions.
- An introduction to
    - Group theory
    - Techniques of approximation including perturbation theory

Types of instruction

The course is structured as a seminar series, where each student is given a specific topic to prepare for a specific seminar. At the seminar the presenting student holds a lecture on the topic, and discuss and frame the topic in view of the learning objectives of the course. Preparation, active participation and attendance (> 80%) are required from fellow students.

In connection to each seminar a set of exercises/problems are handed out, to be handed in in time for the subsequent seminar. Some tasks are to be solved analytically, while some requires computational methods. Teamwork is encouraged when working with the assignments, although individual handing in is requested.

Language of instruction
The course is given in English.

Grades

The grade Pass (G) or Fail (U) is given in this course.

Types of assessment

Assessment is based on

1. The demonstrated knowledge and understanding, as well as pedagogical approach, when holding the seminar. Grading scale: Fail, Pass.
2. Active participation demonstrated by insightful questions and critical reasoning at fellow student's seminars. Grading scale: Fail, Pass.
3. Total grades on handed in assignments: Fail (< 50%), Pass (>50%)
4. Attendance on seminars, > 80% required to Pass

In order to pass the course, all four modules have to be passed.

Students who fail a module will be offered another opportunity to complement the module, no later than three months after final course occasion.

Course evaluation

The students will at the final course occasion be given the opportunity to give feedback on the course. The format of the course evaluation is an interactive questionnaire combining anonymous answers with a general discussion and reflection on the course.

The results of the evaluation are summarised and made available at the course Canvas page. The students will be informed of the results and any decisions that are made based on the course evaluations.

KEM131 Kolloid- och ytkemi, 15 högskolepoäng

Colloid and Surface Chemistry, 15 credits

Avancerad nivå / Second Cycle

Fastställande

Kursplanen är fastställd av Institutionen för kemi och molekylärbiologi 2014-02-12 och senast reviderad 2022-09-14. Den reviderade kursplanen gäller från och med 2022-09-14, vårterminen 2023.

Utbildningsområde: Naturvetenskapligt 100 %
Ansvarig institution: Institutionen för kemi och molekylärbiologi

Inplacering

Kursen ges inom Kemi, masterprogram samt som fristående kurs. Kursen ersätter kurs KEM130 och kurserna kan inte räknas samtidigt i en examen.
Kursen är inplacerad på nivån 120-180 högskolepoäng för kandidatexamen och räknas som kurs på avancerad nivå för masterexamen.

Kursen kan ingå i följande program: 1) Atmospheric Science, Master Program (N2ATM), 2) Kemi, masterprogram (N2KEM), 3) Läkemedelskemi, kandidatprogram (N1LMK) och 4) Kemi, kandidatprogram (N1KEM)

Huvudområde	*Fördjupning*
Kemi	A1N, Avancerad nivå, har endast kurs/er på grundnivå som förkunskapskrav

Förkunskapskrav

För tillträde till kursen krävs avslutade och godkända kurser om 120 hp inom det naturvetenskapliga fältet. Inom ramen för kursfordringarna rekommenderas godkända kurser KEM040 Fysikalisk kemi (15 hp) och MMGK11 Naturvetarmatematik A1 (15 hp) eller motsvarande kunskaper.

Lärandemål

Efter genomgången kurs förväntas studenten kunna:

Kunskap och förståelse

- **Definiera och diskutera** ytspänning och ytfastermodynamik,
- **beskriva** tensiders självassociation och deras betydelse för emulsioner, mikroemulsioner, skum och flotation,
- **beskriva** växelverkan i kolloidala system och dess betydelse för kolloidala systems stabilitet,
- **redogöra** för transportfenomen: viskositet, diffusion, sedimentation och elektrokinetiska fenomen.

Färdigheter och förmåga

- **Karakterisera** kolloidala systems egenskaper,
- **utföra** beräkningar av olika egenskaper hos kolloidala system med hjälp av enkla approximativa teorier.

Värderingsförmåga och förhållningssätt

- **Tolka** kolloidala systems egenskaper med hjälp av grundläggande teorier,
- kritiskt **utvärdera** litteratur inom kolloid- och ytkemi.

Innehåll

Kursen behandlar kolloid- och ytkemi ur ett fysikalisk-kemiskt perspektiv.

Delkurser

1. **Teori** *(Theory),* 9 hp

   Betygsskala: Väl godkänd (VG), Godkänd (G) och Underkänd (U)
   I delkursen *Teori* behandlas följande ämnen:

   1. Fasgränsfenomen: Ytspänning, ytfastermodynamik, Gibbs adsorptionsisoterm, Youngs ekvation, Young-Laplace-ekvationen och monoskikt.
   2. Kolloidal växelverkan och stabilitet: Grundläggande elektrostatik, elektriska dubbelskikt, van der Waals-växelverkan, DLVO-teori samt elektrostatisk och sterisk stabilisering.
   3. Tensider i vattenlösning: Miceller, kritisk micellbildningskoncentration, flytande kristallina faser, mikroemulsioner, emulsioner, skum och flotation.
   4. Transportfenomen: Viskositet, Brownsk rörelse och diffusion, Ficks lagar, Stokes-Einstein-formeln, sedimentation, elektrokinetiska fenomen inklusive elektrofores och elektroosmos, Smoluchowskis och Hückels ekvationer.
   5. Metoder att karakterisera kolloidala system: Viskosimetri, mikroelektrofores, sedimentationsmätningar, ytspänningsmätningar, statisk och dynamisk

ljusspridning.
6. Laborationer:

2. **Laborationer** *(Laboratory Work),* 6 hp
Betygsskala: Godkänd (G) och Underkänd (U)
Laborationerna berör följande ämnen:

- Ytspänning,
- kolloidal stabilitet,
- diffusion,
- mikroelektrofores.

Former för undervisning

Delkurs 1: Undervisningen sker i form av föreläsningar och övningar.

Delkurs 2: Undervisningen sker i form av laborationer inklusive skriftliga redovisningar. Laborationerna är obligatoriska.

Undervisningsspråk: engelska och svenska
Kursen ges som huvudregel på engelska men kan ges helt eller delvis på svenska om omständigheterna påkallar det.

Former för bedömning

Delkurs 1: Kunskapskontroll sker genom skriftlig salstentamen vid kursens slut.

Delkurs 2: Kunskapskontroll sker fortlöpande genom laborationsredovisningar.

För student som ej blivit godkänd vid ordinarie prov erbjuds ytterligare provtillfällen.

Om student som underkänts två gånger på samma examinerade moment önskar byte av examinator inför nästa examinationstillfälle, ska sådan begäran inlämnas skriftligt till institutionen och bifallas om det inte finns särskilda skäl däremot.

I det fall en kurs har upphört eller genomgått större förändringar ska studenten i normalfallet garanteras tillgång till minst fyra provtillfällen (inklusive ordinarie provtillfälle) under en tid av åtminstone två år med utgångspunkt i kursens tidigare uppläggning.

Betyg

På kursen ges något av betygen Väl godkänd (VG), Godkänd (G) och Underkänd (U).
Delkurs 1: betyg bestäms av den skriftliga tentamen.

Delkurs 2: för betyg G krävs aktivt deltagande och godkända labrapporter i samtliga laborationer.

Slutbetyg: För betyg G krävs betyg G på båda delkurser. För betyg VG krävs betyg VG på delkurs 1 och betyg G på delkurs 2.

Angående tillämpning av ECTS-skalan för betyg var god se Rektors beslut 2007-05-28, dnr G 8 1976/07.

Kursvärdering

Kursvärdering görs i relation till kursens lärandemål och innehåll och genomförs i slutet av kursen genom en individuell skriftlig enkät på Göteborgs universitets lärplattfrom. Student som deltar i eller har avslutat en kurs ska ges möjlighet att anonymt framföra erfarenheter av och synpunkter på kursen i en kursvärdering. En sammanställning av kursvärdering och kursansvarig lärares reflektion ska tillgängliggöras för studenterna inom rimlig tid efter kursslut.

KEM170

Advanced Atmospheric Chemistry (7.5hp)

This is a specialized course that focuses on reviewing current cutting edge research, using a series of "atmospheric chemistry" reviews published by Chemical Society Reviews. Students should have some foundational background in heterogeneous chemistry and atmospheric behavior. Thus, this Ph.D course will largely build upon introductory level courses, e.g., the undergraduate and master level "Atmospheric Chemistry" course or equivalent experience. The course will be structured as a moderated discussion with each student being expected to give 1-2 detailed presentations from the literature. Each presentation will be focused on a single review paper and the student presentations will be used to stimulate a peer-discussion regard- ing the most relevant research questions in the field and sub-fields. Students will be expected to prepare for the discussions with a critical eye, as if they were being consulted in the peer- review process. Senior researchers from various sub-fields will be invited to participate in the discussion and guest researchers will visit to present lectures and augment the discussions.

In addition to exploring a broad range of cutting edge contemporary research questions, this course will help to develop the presentation and critical thinking skills of the students. In ad- dition to presenting material students will be expected to participate in peer-to-peer critical discussions.

Course Instructors:

•Dr. Erik S. Thomson (erik.thomson@chem.gu.se) •Dr. Ravi Kant Pathak (ravikantpathak@gmail.com)

Course Meetings and Evaluation:

The course will meet approximately once per week (2 hours) beginning in late April. There will be a total of 15-17 meetings with a break during summer vacations. The first meeting, which will be largely organizational, will take place Thursday, April 18 at 1400, in the coffee room of Atmospheric Sciences. At this first meeting the instructors will present relevant background material and the regular time/place of the course meeting will be agreed upon. To encourage

dynamic discussions course meetings will be open to any interested participant, and an effort will be made to include senior researchers in topical areas. Additionally, a video conferencing connection may be made available to students outside of Gothenburg.

Student evaluations will be based on: (1) student presentations, (2) participation in course dis- cussions, and (3) an end of course oral examination. The oral exam will be a short 25 minute discussion between the instructors and individual students. It will focus on the major research questions in the series of reviews presented during the course. At the end of the exam 5 minutes will be reserved for feedback to the instructors. Students will be given pass/fail marks.

To Apply:

Applications should be made by joint email to the course instructors. In your application for this course please indicated your (1) department and area of research, including your current research topic, (2) supervisors name, and (3) your year of study.

DEPARTMENT OF CHEMISTRY AND MOLECULAR BIOLOGY

KEM552 Introduction to molecular modelling, 5 credits

Grundläggande molekylmodellering, 5 högskolepoäng

Second Cycle

Confirmation

This course syllabus was confirmed by Department of Chemistry and Molecular Biology.

Field of education: Science 100%
Department: Department of Chemistry and Molecular Biology

Position in the educational system

The course is classified at the level 90-120 credits for Degree of Bachelor. Alternatively, it can be read as a course at second cycle level for Degree of Master (120 credits) or as a freestanding course for PhD students. The course replaces the earlier courses KEM551 and KEN550 and can not be included together with one of them in the same degree.

The course can be part of the following programmes: 1) Chemistry and learning, Master's Programme (N2KOL), 2) Master's Programme in Organic and Medicinal Chemistry (N2KEL), 3) Master's Programme in Chemistry (N2KEM), 4) Bachelor of Science Programme in Medicinal Chemistry (N1LMK); 5) Bachelor of Science Programme in Chemistry (N1KEM); 6) Part of a PhD-level education.

Main field of studies

Chemistry

Chemistry with Specialization in Medicinal Chemistry

Entry requirements

Specialization

A1N, Second cycle, has only first-cycle course/s as entry requirements

A1N, Second cycle, has only first-cycle course/s as entry requirements

For admission to the course, completed and approved courses worth 90 credits in the field of science (or 120 credits in pharmaceutics/medicine) are required. Completed course KEM040, Physical Chemistry (15 credits), or FYP203, Quantum Physics A (7.5 credits) or equivalent knowledge, as well as knowledge equivalent to at least course MMGK11, Mathematics for natural scientists A1 (15 credits) are recommended.

Learning outcomes

After completion of the course the student is expected to be able to:

Knowledge and understanding

- **present** the basic ideas of molecular modelling and its importance to solve chemical problems, **describe** applications of molecular mechanics in different fields of chemistry,
- **explain** the idea behind molecular mechanics and the structure of a force field, **name** the different types of force fields and **explain** the meaning and structure of the terms in a force field,
- **name** some important available force fields, their properties and areas of application,
- **describe** different methods to find the equilibrium geometries of a system,
- **explain** the principle behind the molecular dynamics (MD) and Monte-Carlo (MC)

  methods as well as areas of application for these methods.

  Competence and skills

- **build** molecule models with the program packages Molecular Operating Environment and Chimera,
- **set up** and **carry out** energy minimisations,
- **set up**, **carry out** and **evaluate** simple docking protocols,
- **set up** MC and MD calculations in an appropriate way and analyse result from these

  calculations,

- **use** visualisation methods efficiently.

Judgement and approach

• **assess** quality and reliability of computational results and **decide** in which cases molecular mechanics is sufficient.

Course content

The course describes the molecular modelling with a focus on molecular mechanics, which is the appropriate method to study large systems (e g proteins or DNA molecules) under realistic conditions (aqueous solution, finite temperature). The following subjects will be treated:

1. The standard tools of molecular modelling: Molecular mechanics, force fields, types of force fields
2. Finding equilibrium structures: Geometry optimisation
3. Simulations under real conditions: Molecular dynamics (MD) and Monte-Carlo (MC) methods
4. Conformation search
5. Visualisation and molecular properties
6. Applications of molecular modelling: Simulation of large molecules, ligand-receptor docking, pharmacophoric modelling
7. Trends in molecular modelling: Polarisable force fields, force fields for chemical reactions, QM/MM,...

The lectures are accompanied by computer-based laboratory sessions where important topics of the theory are demonstrated and are trained based on modern program packages. The final part of course includes a shorter computational project that the student implements, summarises in a report, and present in class.

The course is divided into two modules. Module 1 (3.0 credits) includes the theory as above, module 2 (2.0 credits) includes the laboratory sessions.

Sub-courses

1. **Theory part *(Teoridelen),* 3 credits**

   Grading scale: Pass with Distinction (VG), Pass (G) and Fail (U)

2. **Computer exercises *(Datalaborationer),* 2 credits Grading scale: Pass (G) and Fail (U)**

Form of teaching

Module 1: Teaching is performed in the form of lectures as well as a project work.
Module 2: Teaching is performed in the form of computer-based laboratory sessions

including presentations.

Language of instruction: English and Swedish
As a principal rule, the course is given in Swedish but can be given completely or partly in English if the circumstances require it.

Assessment

Module 1: The examination is done by implementation and presentation of project work.

Module 2: The examination is done based on active participation in laboratory sessions and presentations.

If a student who has failed the same examined component twice wishes to change examiner for the next examination, a written application shall be sent to the department responsible for the course and it shall be granted unless there are special reasons against (Chapter 6, Section 22, Higher Education Ordinance).

In case a course has been discontinued or has undergone major changes, the student will normally be guaranteed at least three opportunities to take the examination (including the ordinary examination) during a period of at least one year from the last time the course was given in its original form.

Grades

The grading scale comprises: Pass with Distinction (VG), Pass (G) and Fail (U).
Module 1: Grade Pass with distinction, Pass or Fail will be awarded.

Module 2: Grade Pass or Fail will be awarded.

Final grade: For grade of Pass on the whole course, grades of Pass on module 1 and Pass on module 2 are required. For grade of Pass with distinction on the whole course, grade of Pass with distinction on module 1 and Pass on module 2 are required.

Course evaluation

Course evaluation is done in relation to the intended learning outcomes and content of the course and is carried out at the end of the course by an individual written questionnaire on University of Gothenburg's virtual learning environment. A student who participates in, or has completed, a course should be given he opportunity to

anonymously express experiences of and views on the course in a course evaluation. A compilation of the course evaluation along with reflections by the responsible teacher should be made available for the students within reasonable time after the end of the course.