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Faculty Board

# General Syllabus for Third-Cycle Studies in Theoretical Chemistry, NAKEMTK2

This syllabus was approved by the Board of the Faculty of Science on 12 June 2019 and applies to third-cycle students admitted from 1 July 2019.

The syllabus is based on the Higher Education Ordinance (1993:100) Chapter 6 Sections 1–11, 25–36, Chapter 7 Sections 34–41 and Annex 2 Qualifications Ordinance.

# 1. Available degrees

The programme described in this syllabus can lead to one of the following degrees:

Doctor of Philosophy in Theoretical Chemistry Licentiate of Philosophy in Theoretical Chemistry

In consultation with the Faculty of Engineering/LTH, the Faculty Board has decided (NA35 643/2005) that students admitted to third-cycle studies at the Faculty of Science on the basis of an MSc in Engineering shall be entitled to be awarded the degrees of Doctor of Philosophy in Science or Licentiate of Science without special application.

# 2. Subject description

Research in Theoretical Chemistry entails the development of quantum chemistry and statistical-mechanical methods to describe chemical systems and processes. These methods are applied to solve or illuminate questions primarily in surface chemistry and polymer chemistry, biochemistry, intermolecular interaction and spectroscopy.

# 3. Objectives

Third-cycle courses and study programmes shall be based fundamentally on the knowledge acquired by students in first- and second-cycle courses and study programmes, or its equivalent. In addition to the requirements for first- and second-cycle courses and study programmes, third-cycle courses and study programmes shall develop the knowledge and skills required to be able to undertake autonomous research. It is also desirable for doctoral students to acquire teaching experience.

The general outcomes for third-cycle courses and study programmes are defined in the Higher Education Ordinance Annex 2 Qualifications Ordinance.

# 3.1. Learning outcomes for a degree of Doctor

#### Knowledge and understanding

For the degree of Doctor the third-cycle student shall

- demonstrate broad knowledge and systematic understanding of the research field as well as advanced and up-to-date specialised knowledge in a limited area of this field, and
- demonstrate familiarity with research methodology in general and the methods of the specific field of research in particular.

### Competence and skills

For the degree of Doctor the third-cycle student shall

- demonstrate the capacity for scholarly analysis and synthesis as well as the ability to review and assess new and complex phenomena, issues and situations autonomously and critically
- demonstrate the ability to identify and formulate issues with scholarly precision critically,
  autonomously and creatively, and to plan and use appropriate methods to undertake research and other
  qualified tasks within predetermined time frames and to review and evaluate such work
- demonstrate through a thesis the ability to make a significant contribution to the formation of knowledge through his or her own research
- demonstrate the ability in both national and international contexts to present and discuss research and research findings authoritatively in speech and writing and in dialogue with the academic community and society in general
- demonstrate the ability to identify the need for further knowledge, and
- demonstrate the capacity to contribute to social development and support the learning of others both through research and education and in some other qualified professional capacity.

### Judgement and approach

For the degree of Doctor the third-cycle student shall

- demonstrate intellectual autonomy and disciplinary rectitude as well as the ability to make assessments of research ethics, and
- demonstrate specialised insight into the possibilities and limitations of research, its role in society and the responsibility of the individual for how it is used.

# 3.2. Learning outcomes for a degree of Licentiate

#### Knowledge and understanding

For a degree of Licentiate the third-cycle student shall

 demonstrate knowledge and understanding in the field of research including current specialist knowledge in a limited area of this field as well as specialised knowledge of research methodology in general and the methods of the specific field of research in particular.

# Competence and skills

For a degree of Licentiate the third-cycle student shall

demonstrate the ability to identify and formulate issues with scholarly precision critically, autonomously and creatively, and to plan and use appropriate methods to undertake a limited piece of research and other qualified tasks within predetermined time frames in order to contribute to the formation of knowledge as well as to evaluate this work

- demonstrate the ability in both national and international contexts to present and discuss research and research findings in speech and writing and in dialogue with the academic community and society in general, and
- demonstrate the skills required to participate autonomously in research and development work and to work autonomously in some other qualified capacity.

# Judgement and approach

For a degree of Licentiate the third-cycle student shall

- demonstrate the ability to make assessments of ethical aspects of his or her own research
- demonstrate insight into the possibilities and limitations of research, its role in society and the responsibility of the individual for how it is used, and
- demonstrate the ability to identify the personal need for further knowledge and take responsibility for his or her ongoing learning.

# 4. Admission requirements

The requirements for admission to third-cycle courses and study programmes are that the applicant meets the general and specific entry requirements, and is considered in other respects to have the ability required to benefit from the course or study programme.

## General admission requirements

A person meets the general entry requirements for third-cycle courses and study programmes if he or she:

- 1. has been awarded a second-cycle qualification, or
- 2. has satisfied the requirements for courses comprising at least 240 credits, of which at least 60 credits were awarded in the second cycle, or
- 3. has acquired substantially equivalent knowledge in some other way in Sweden or abroad.

The head of department may permit an exemption from the general entry requirements for an individual applicant, if there are special grounds.

# Specific admission requirements

A minimum of 120 credits are to derive from chemistry courses, of which at least 30 credits from a second-cycle degree project in the chosen specialisation or a closely related specialisation.

In certain cases, the requirement for chemistry courses may be replaced by other subjects. Sixty credits in physics and 60 credits in mathematics also meet the requirements for Theoretical Chemistry.

The specific admission requirements can also be fulfilled through another equivalent programme, which is assessed in each specific case.

# 5. Selection

In selecting between applicants who meet the requirements, their ability to benefit from the course or study programme shall be taken into account. However, the fact that an applicant is considered able to transfer credits from prior courses and study programmes or for professional or vocational experience may not alone give the applicant priority over other applicants.

The following selection criteria will be applied:

Study record from undergraduate and Master's courses or the equivalent.

The breadth, depth and relevance of undergraduate and Master's courses or the equivalent.

The quality of the degree project and other independent work.

Other knowledge and skills of relevance to the research specialisation.

Suitable candidates should be called to an interview, if possible.

The recruitment and selection to third-cycle studies must always take diversity and gender balance into account, in compliance with the Lund University gender equality policy, equal opportunities policy and diversity plan. The underrepresented gender should always be given precedence in cases of equal qualifications, unless there are valid reasons to the contrary.

Furthermore, it must be possible to match the student's research interests with the supervisory resources available at the department.

# 6. Degree requirements

The completion of the third-cycle programme results in a degree of Doctor of Philosophy or, if the student so wishes or if this is stated in the admission decision, a degree of Licentiate. The student may also but is not obliged to complete a degree of Licentiate as a stage in the third-cycle programme.

The degree of Doctor comprises 240 credits and the degree of Licentiate 120 credits.

#### 6.1. Thesis

The programme is to include a research project documented in a PhD or Licentiate thesis. The thesis is to be defended orally at a public defence and reviewed by an external reviewer (PhD thesis) or critical reviewer (Licentiate thesis).

## PhD thesis

The PhD thesis is to comprise a minimum of 150 credits.

The PhD thesis may be structured as a compilation thesis or a monograph thesis.

A compilation thesis consists of copies of a number of research articles or manuscripts and a summarising chapter. The articles may be written by the doctoral student individually or in cooperation with others, but the summarising chapter must be written individually by the doctoral student. The research articles must be of a quality required for publication in recognised peer-reviewed journals and it must be possible to distinguish the contributions of different authors. At least two articles, or equivalent, should be accepted for publication by recognised research journals. The summarising chapter is to consist of an introduction to the research area of the thesis and a presentation and discussion of the findings of the articles. The presentation and discussion shall be written in a form and style that is independent and different from the articles. This makes it possible to situate the findings in a wider context.

A monograph thesis is a unified report including descriptions of the research issue, research questions, methods, analysis, findings and discussion.

#### Licentiate thesis

The Licentiate thesis is to comprise a minimum of 90 credits.

The Licentiate thesis can be designed as a summary of at least one research article (or manuscript), written by the student individually or in cooperation with others, or a unified research report (monograph). The thesis must be of a quality required for publication in recognised peer-reviewed journals and it must be possible to distinguish the contributions of different authors. For more information on summary and monograph theses, please see compilation thesis and monograph thesis above.

# 6.2. Courses and other programme components

The courses and other components of the third-cycle programme in Theoretical Chemistry are to comprise 45–90 credits for a degree of Doctor and 10–30 credits for a degree of Licentiate. The exact extent of the credit requirement in addition to the thesis is to be stated in the individual study plan. Specialised courses in Theoretical Chemistry are to account for at least 30 credits in third-cycle studies or equivalent.

Courses or other credit-earning components included in the programme can be completed both within and outside Lund University. For courses or other programme components taken outside the Faculty of Science, the number of credits to be transferred is decided by the head of department (can be delegated).

The following courses are compulsory:

- Introductory course worth at least 1.5 credits, of which 0.5 credits is to be made up of the faculty-wide introductory course for doctoral students
- Work environment, environmental considerations and risks, 2 credits
- Research ethics for chemists, 2 credits, or equivalent course
- Doctoral students who teach are to complete the basic teaching and learning course worth 3 credits.