LUNDS UNIVERSITET

NATUR-
VETENSKAPLIGA
FAKULTETEN

SYLLABUS

Reg. no
U 2024/66

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Faculty Board

General syllabus for third-cycle studies in Computational Chemistry, NAKEMT02

This syllabus was approved by the Faculty Board on 14 February 2024. It replaces NAKEMT01 and applies to doctoral students admitted from 15 February 2024.

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

1. Available degrees

Studies in line with this general syllabus can lead to one of the following degrees:

Doctor of Philosophy in Computational Chemistry / *Filosofie doktorsexamen i beräkningskemi*

Licentiate of Philosophy in Computational Chemistry / *Filosofie licentiatexamen i beräkningskemi*

In consultation with the Faculty of Engineering, LTH, the Faculty Board has decided (NA35 643/2005) that those who have been admitted to third-cycle studies at the Faculty of Science with a Degree of Master of Science in Engineering as a qualifying criterium can be given the title of Doctor of Philosophy in Engineering or Licentiate of Philosophy in Engineering without special assessment.

2. Subject description

In many scientific fields, computation has become such an important part of the research that it has developed into a branch of its own within the field, for example, computational chemistry within chemistry. Computational science is a collective term for such activities within different disciplines.

Computational science is in the broadest sense research using or developing digital tools for advanced computation or data management. Such research activities can be simulation and modelling as well as research data analysis and handling. This also includes the development of models, methods, software, utilities, frameworks and databases. This broad definition is also covered by the term e-science.

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

3. Objectives

Third-cycle courses and study programmes are to be based fundamentally on the knowledge acquired by students during first and second-cycle courses and study programmes, or the equivalent. In addition to what applies to first and second-cycle level education, third-cycle education is to develop specific knowledge and skills needed to be able to conduct independent research. It is also desirable for the doctoral student to acquire teaching experience.

The overall objectives for third-cycle education are defined in Annex 2 of the Higher Education Ordinance, the Qualifications Ordinance.

3.1. Learning outcomes for a Degree of Doctor

Knowledge and understanding

For a Degree of Doctor the doctoral 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 a Degree of Doctor the doctoral student shall

– demonstrate the capacity for scholarly analysis and synthesis as well the capacity 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 advanced 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 their 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 advanced professional capacity.

Judgement and approach

For a Degree of Doctor the doctoral 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 doctoral 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 doctoral 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 advanced 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 advanced capacity.

Judgement and approach

For a Degree of Licentiate the doctoral student shall

– demonstrate the ability to make assessments of ethical aspects of their 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 their personal need for further knowledge and take responsibility for their ongoing learning.

4. Entry requirements

The requirements for entry to third-cycle studies 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 programme.

General entry requirements

A person meets the general entry requirements for third-cycle studies if the individual

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 can permit an exemption from the general entry requirements for an individual applicant, if there are special grounds.

Specific entry requirements

At least 120 credits are to consist of chemistry courses, of which at least 30 credits from a second-cycle degree project within the chosen specialisation or closely related specialisations.

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 entry requirement may also have been obtained through other equivalent education, which is assessed in each individual case.

5. Selection

In selecting between applicants who meet the requirements, their ability to benefit from the course or study programme is to be

taken into account. 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 principles are applied:

Results achieved in first and second-cycle (or equivalent) courses and study programmes. Broad, deep and relevant expertise from first and second-cycle (or equivalent) courses and study programmes. The quality of the degree project and other independent projects.

Other expertise or skills that are relevant to the chosen research specialisation.

Applicants who appear to be well-suited should, whenever possible, undergo an interview.

When recruiting and selecting students for third-cycle education, diversity and an even gender distribution must always be taken into account in accordance with Lund University's gender equality policy, equal opportunities policy and diversity plan. The under-represented gender is to be given priority among equally qualified candidates, unless special reasons dictate otherwise.

There must also be coherence between the student's research interests and the department's ability to provide competent supervision.

6. Degree requirements

The third-cycle study programme ends with a Degree of Doctor or, if the doctoral student so wishes or if this has been stated in the admission decision, with a Degree of Licentiate. The doctoral student is also entitled, but not obliged, to take a Degree of Licentiate as a stage in the education leading to a Degree of Doctor.

The Degree of Doctor comprises 240 credits while the Degree of Licentiate comprises 120 credits.

6.1. Thesis

The programme must include a research project documented in a doctoral or licentiate thesis. This project is to be defended at a public defence (Degree of Doctor) or a public seminar (Degree of Licentiate), in both cases with a reviewer.

Doctoral thesis

The thesis is to comprise at least 165 credits.

The doctoral thesis is to be a carefully thought-out and reasoned discussion of the candidate's own work in relation to the broader research area, and can be produced either as a *compilation thesis* or a *monograph.*

A compilation thesis consists of attached copies of a number of research articles or manuscripts, along with a summarising chapter. The research articles are to be of a quality corresponding to the requirements for publication in recognised academic journals with peer review procedures, and it should be possible to distinguish the doctoral student's contribution in the work.

It is rarely the case that the research papers in a compilation thesis are solely authored by the doctoral student. For this reason, importance should be attached to the summarising chapter that in part gives the doctoral student the opportunity to display an independent intellectual performance and in part enables assessment of the doctoral student's independent contributions. The summarising chapter is to provide an introduction to the papers and place the issues and results achieved into an overall context. The summarising chapter must therefore be written in a different format to the papers in the thesis, and it must be possible to read it as an independent academic text. The summarising chapter must not contain extensive copying of text, figures and tables from the constituent parts.

The monograph comprises a cohesive report detailing research tasks, issues, working methods, analysis, results and discussion. For monographs, it is particularly important that the candidate's own research is presented in such a way that the methods used,

results achieved and conclusions drawn can be understood and assessed.

The thesis must relate to the Higher Education Ordinance's formulation of learning outcomes, which means the objectives of both the compilation thesis and the monograph are principally to:

- demonstrate current specialist knowledge and a broad and deep understanding of the research area
- demonstrate the ability to place the thesis into a broader theoretical and research context
- express clear objectives of the thesis and its most important hypotheses and issues
- demonstrate familiarity with the methods and analytical tools used within the research area, and demonstrate an ability to assess and evaluate them
- demonstrate an ability to reflect on the importance and limitations of the candidate's own research
- make a significant contribution to expanding knowledge in the field and identify needs for more knowledge.

The thesis must contain a popular science summary, which can be written in Swedish or English.

Licentiate thesis

The thesis is to comprise at least 82,5 credits.

The licentiate thesis can be designed either as a summary of at least one academic article (or manuscript), which the doctoral student has written alone or jointly with others, or as a uniform, coherent academic work (monograph). The licentiate thesis is to be of a quality corresponding to the requirements for publication in recognised academic journals (with peer review procedures), and it is to be possible to distinguish the various authors' contributions in the work. For details regarding the summary and monograph, see the compilation thesis and monograph section above.

6.2. Courses and other credit-earning components

The courses and other components of the third-cycle programme in computational chemistry are to comprise 60–75 credits for a

Degree of Doctor and 30–37.5 credits for a Degree of Licentiate. The exact scope of the credit requirement in addition to the thesis project is to be specified in the individual study plan. Subject-specific courses in computational chemistry are to account for at least 30 third-cycle credits or equivalent for a Degree of Doctor and 15 credits for a Degree of Licentiate.

Courses or other credit-earning components that are included in the programme may be completed both at or outside Lund University.

Compulsory courses and other credit-earning components

– Introduction to the Department (at least 1 credit)
– Faculty-wide Introductory Course for Doctoral Students (0.5 credits)
– Work Environment, Environmental Considerations and Risks (2 credits)
– Research Ethics (3 credits)

Doctoral students who teach are to undergo basic training in teaching and learning in higher education (3 credits).