Theoretical Chemistry and Biology

Study plan for third-cycle subject

The subject plan was approved by Fakultetsnämnden (Faculty Board) January 25, 2011. Valid from Spring 11.

Subject title

Theoretical Chemistry and Biology (Teoretisk kemi och biologi)

Subject description and programme outcomes

Scientific field

Theoretical Chemistry and biology is an interdisciplinary research field where physics, mathematics and computer science are used to examine, explain and anticipate chemical and biological phenomena and processes including the properties of different materials.

Description of possible specialisation

The subject has no specialisations.

Specification of how the programme outcomes are to be achieved

The general aim and the goals for doctoral program in Biotechnology is in agreement with the guidelines for third-cycle courses and study programmes that has been established by KTHs Faculty board:

• The aim of research level (third-cycle) education of KTH is to provide society with qualified researchers that can contribute to a sustainable development of the society.
• The goal of KTH's education for third-cycle studies is that the doctoral students should become independent, excellent researchers.

The research level (third-cycle) students should, after completed studies, be able to:

• describe and explain theories and empirical results in his/her field of research.
• formulate specific research issues in this field of research.
• use scientific methods and develop new knowledge through his/her own scientific studies.
• critically analyse and evaluate methods applied and results from his/her own scientific studies and those of others.
• present and discuss research results in the scientific community.
• present research in a pedagogical manner outside the scientific community, and also in an educational context.
• assess ethical aspects of research within the current field and act from these and
• identify the need for new knowledge and have knowledge of how to initiate and lead research

Apart from these aims are specific aims for this third-cycle subject area. After completed education, the student should have the following skills in the stated fields:

Knowledge and understanding

• Have a broad disciplinary foundation to be able to work in the fields in theoretical chemistry and biology or general mathematical modelling. This knowledge should include basic skills in programming, knowledge of numerical mathematical methods and different applications against chemical or biological problems.
- Show a broad knowledge in the area including knowledge of data modeling and natural sciences and especially deep knowledge in certain parts of the field.

Skills and skill

- Show on a good ability to, independently of others as well as in groups, apply knowledge and skills in practical action with consideration taken to relevant scientific and social assessments and positions.
- Be capable to define clear scientific issues plan for how a problem can be solved and hold necessary skill to solve research issues in theoretical chemistry and biology.
- Possess individual and professional skills such as language fluency, leadership skill, project management and communication ability in order to work as researchers in a research oriented company, as a research head in a technology-intensive company, or to be able to continue toward an academic research career.

Judgement ability and attitude

- Possess a very good understanding that research questions are often very complex, not always be completely defined and sometimes imply a conflict between aims and preconditions.
- Show an understanding of the responsibility and the ethical considerations that can arise in connection with different technical, organisational, economic, ecological and social activities.

Current research

Issues in the subject area concern basic concepts and methods in Theoretical Chemistry and biology as well as important application fields as chemical catalysis for long-term energy conversion, atmospheric chemistry, nanobiotechnology, enzyme catalysis, drug development, design and visualisation of biomolecules, protein dynamics, and properties of modern "soft" materials in general.

Programme structure

The education for third-cycle studies in Theoretical chemistry and biology contains both a course module and a dissertation. Courses are classified as advanced courses, skills courses, broadening courses or other courses. Certain courses are compulsory for all students in Theoretical chemistry and biology. Courses can be arranged by home university (KTH) or some other national or international university, institute or company. Observe that the quality and the level of courses that are arranged by other organisations than universities must be reviewed and be accepted by the director of third-cycle education (forskarutbildningsansvarig) before these can constitute a part of the course block in an individual study plan. In those cases where a Degree of Licentiate is not the end goal, it is recommended that a 2-year seminar (2-Års-seminarium) be held by the student after approximately 20-26 months of studies, at which so-far achieved results are described, including both the dissertation as well as the course module, as well as that a general plan over the continuation of the studies is presented. Two senior researchers are appointed as reviewers and participate at a follow-up meeting, together with the student the principal supervisor and assistant supervisor, and hold a constructive discussion of the planning of the continued studies toward Degree of Doctor.

The dissertation portion of the education is based on an accumulation of own theoretical and/or experimental data in the research field that leads to the completion of a written thesis that can be defended at a public defence of doctoral thesis at the end of the third-cycle courses and study programmes (see section 5). The education takes place under supervision by a principal supervisor together with one or or several assistant supervisor in agreement with a so called Individual Study plan (ISP) which be updated at least once a year (or more often when necessary) and that should be accepted by the director of third-cycle studies (forskarutbildningsansvarig).

Compulsory and recommended courses

A Degree of Licentiate includes a course module of at least 30 credits and a dissertation portion equivalent to 90 credits that together constitute an education of 120 credits (equivalent to two years of full-time studies). At least 50% of the credits (15 credits) should be constituted by courses for third-cycle studies.

A Degree of Doctor includes a course module of at least 60 credits and a dissertation portion equivalent to 180 credits that together constitute an education of 240 credits (equivalent to four years of full-time study). At least 60% of the credits (= 36 credits) should be constituted by courses for third-cycle studies.
L= Compulsory courses for Degree of Licentiate
D= Compulsory courses for Degree of Doctor

Advanced courses

Theoretical Chemistry and biology

Course code Course name Credit

NM: MC3 Mathematical and numerical methods for chemists and biologist 10 R
FBB3030 Computer-based chemistry 8 O (L/D)
FBB3060 Molecular modelling, basic applications 8 O (L/D)
FBB3050 Thermodynamics and Statistical Mechanics 10 O (D)
FBB3050 Thermodynamics and Statistical Mechanics 10 O (D)
BB3060 Protein physics 5 R
FBB3060 Molecular Dynamics and Monte Carlo methods 7.5 R
FÅ£A5708 Computer-based Enzymology 5 R
NM:OC10 Multi-scale modelling 10 R
NM:OC8 Computer-based nanotechnology and bio-nanotechnology 10 R
DD2397 Bioinformatics 7.5 R
KJE-3104 Relativistic quantum chemistry 10 R
NM:OC6 Molecular properties 8 R
XXX Protein- (biomolecular) visualisation and haptik 5 R
26 credits as O

Skill courses

Theoretical Chemistry and biology

BB3110 Programming 5 R
1N5113 Theory, Research and Development, technology and scientific specialisation 7.5 O (L/D) Conditional
TBD Element of Scientific computing 5 R
ME2016 Industrial project management 4 R
7.5 credits as O

Broadening courses

Theoretical Chemistry and biology
DD2435 Neural networks 7.5 R
DD2398 Quantitative system biology 3.0 R
TBD Protein visualisation and haptics 3.0 R
2E1395 Pattern Recognition 4 R
0.0 credits as O

Other treatments

Theoretical Chemistry and biology

LH200V Basic communication and learning (GKU) 3.0 O (L/D) Conditional
BB3120 Method in Supervision for project work (R) 6.0 R
3.0 credits as O

**Inclusion of previously read courses**

Under certain conditions, courses that the student has read before admission to third-cycle courses at KTH can be included as part of the course requirements, after approval of the principal supervisor and consulting with KTHs regulatory framework with respect to inclusion of previously read courses. Observe that 60 % of the credits that are required for Degree of Doctor must be courses for third-cycle studies. Inclusion can not be invoked for courses taken that are required for admittance to third-cycle courses and study programmes at KTH.

Further, to be able to profit by the education for third-cycle studies in the specialisation Theoretical Chemistry and biology need students have acquired an advanced knowledge in the subject equivalent (or the equivalent with) the following courses on KTH:

- DD1352 Algorithms, Data Structures and Complexity
- EL1820 Modelling of dynamic system
- MC1 (Masters CCP): Quantum chemistry and physics
- MC2 (Masters CPP): Chemical Kinetics and Dynamics
- MC3 (Masters CCP): Mathematical and Numerical Methods left Chemists
- MC4 (Masters CCP): Scientific programming
- DD2398 Quantitative system biology
- SG1216 Thermodynamics

These so-called "specific entry requirements," concerning courses or other requirements of prior knowledge that are considered necessary to make use of the education for third-cycle studies implies that these courses, or the equivalent such, cannot be counted as part of the individual course block of 60 credits.

**Thesis**

A thesis is a compulsory part of the education for third-cycle studies. As supplements to the general review process on KTH concerning the quality of theses

(see: http://intra.kth.se/regelverk/utbildning-forskning/forskarutbildning/disputation/policy-for-forhandsgranskning-av-doktorsavhandling-licentiatuppsats-1.27246),
should the following criteria, representing an intradisciplinary practice and norm, apply as guidelines for extent and quality for doctor-and licentiate theses. Circumstances that cause these criteria to be considered not applicable or relevant should be discussed with the director of graduate studies and the dean at the School of Biotechnology, KTH.

Doctoral thesis

Compilation thesis

 aç The thesis should normally be based on four articles.

 aç Normally two of the included articles should be either already published or formally accepted for publication ("in press") in international, refereed ("peer reviewed") scientific magazines.

 Other articles may be included as manuscripts sent in for publication ("submitted") in international refereed ("peer reviewed") scientific magazines.

 aç The doctoral student should be first-author on at least two of the included articles, including on one of the articles that belong the category "already have published or accepted for publication".

 aç For all of the included articles should the doctoral student's own contribution be significant and clearly indentifiable.

 aç The thesis should previewed before printing by at least one senior researcher as well as the principal supervisor.

 aç In those cases where a thesis is only based on manuscripts that have not yet been published or accepted for publication ("in press") in international refereed ("peer reviewed") scientific magazines, the thesis and the included manuscripts should be previewed before printing by at least one senior researcher, the principal supervisor, the opponent, and the examining committee.

 Monograph

 aç Monographs should be avoided. KTH has a stated ambition that the contents of theses should be published in international refereed ("peer reviewed") scientific magazines.

 aç The thesis should be previewed before printing by at least two senior researchers, the principal supervisor, and the director of graduate studies.

 Licentiate thesis

 Compilation thesis

 aç The thesis should normally be based on two articles.

 aç Included articles need not be already published or formally accepted for publication ("in press") in international refereed ("peer reviewed") scientific magazines.

 However, normally at least one of the included articles should be sent in for publication ("submitted") in an international refereed ("peer reviewed") scientific magazine.

 aç The doctoral student should emerge as first-author on at least one of the included articles.

 aç For all of the included articles should the doctoral student's own contribution be significant and clearly indentifiable.

 aç If the thesis contains one or more articles that have been published already or been accepted for publication ("in press") in international refereed ("peer reviewed") scientific magazines, the thesis should be previewed before printing by at least one senior researchers as well as the principal supervisor.
Monograph

- If the thesis does not contain an article that has been published already or been accepted for publication ("in press") in international refereed ("peer reviewed") scientific magazines, the thesis should be previewed before printing by at least two senior researchers as well as the principal supervisor.

- Monographs should be avoided. KTH has a stated ambition that the contents of theses should be published in international refereed ("peer reviewed") scientific magazines.

- The thesis should be previewed before printing by at least two senior researchers, the principal supervisor, and the director of graduate studies.

Entry requirements and selection

General and special admission requirements and prior knowledge

Entry requirements to Doctoral program in Biotechnology includes part of the general entry requirements for postgraduate studies described in The Higher Education Ordinance, chapter 7, section 39:

Basic entry requirements are, according to Higher Education Ordinance 7 chapters section 39, one that has:

1. been awarded a second-cycle degree,
2. satisfied the requirements for courses comprising at least 240 credits of which at least 60 credits were awarded in the second-cycle, or
3. In some other way, within or outside the country, acquired equivalent knowledge.

The faculty board may allow exceptions from the general entry requirements for an individual applicant if special circumstances apply.

For entry requirements to the Doctoral Program in Theoretical Chemistry and biology, the above described degree or the advanced courses should be in relevant subject area.

As supplements to these requirements, so-called specific entry requirements can also be made for special focuses. These special requirements include skills necessary to make use of the education and can for example involve knowledge/skills from special fields of importance to the subject area, or linguistic knowledge. The same specific entry requirements apply to students with aims of Degree of Doctor or Degree of Licentiate.

Selection rules and procedures

Selection of students to third-cycle courses and study programmes is first based on if they satisfy the formal requirements for admission. During the application procedure, the applicant's potential to make use of the education is assessed, typically through interviews and an overview of earlier activities, degrees and certificate, but also through an assessment of talent and skill, maturity level, independence, ability to express thoughts in writing and verbally, linguistics and ability for critical thinking. Admission to third-cycle courses and study programmes is made by relevant dean, after assessment from the director of third-cycle studies (forskarutbildningsansvarig) about formal eligibility of the proposed principal advisor and assistant advisor.

The programme’s degrees and examinations

Degree of Licentiate and Degree of Doctor (PhD)

Examination of licentiate and Degree of Doctor are made according to KTHs regulatory framework (see "the KTHhandboken" on http:// intra. kth. see). A Degree of Licentiate can constitute a final examination. Even if a Degree of Doctor constitutes final examination, a Degree of Licentiate can first be issued. In short; apart from completing of a full course block of 30 or 60 credits for licentiate respective Degree of Doctor, a defence of the thesis is also required for both types of degrees, written on the basis of results of theoretical and/or practical studies. A licentiate thesis is
presented at a public seminar. The licentiate thesis should be reviewed by at least a teacher or senior researchers. The principal supervisor decides if the thesis should be accepted or not. A doctoral thesis is defended at a public seminar, where the thesis is reviewed by a peer reviewer as well as an examining committee consisting of three or five members. The examining committee decides if the thesis should be accepted or not.

**The programme’s examinations**

Compulsory courses in the specialisation:

- BB3030 Molecular modelling, Basic tools
- BB3060 Molecular modelling, Basic applications
- BB3050 Molecular modelling, Macroscopic models
- 1N5113 Theory of Science and Research, technology and natural sciences specialisation
- LH200V Basic communication and teaching

Courses in third-cycle courses and study programmes should contain either an oral or written examination. The examiner must in each individual case ensure that the student satisfied the course requirements.