Doctoral programme — Theoretical Chemistry and Biology

Programme description (KTHTKB)

Programme name
Theoretical Chemistry and Biology (Teoretisk kemi och biologi)

Subject area

The doctoral programme’s overall purpose and learning outcomes
The general aim and the aims for Doctoral program in Theoretical Chemistry and biology överensstämmer with the guidelines for third-cycle courses and study programmes that has established by KTHs Faculty board:

â¢ The aim of KTHs education for third-cycle studies is to equip the society with qualified researchers that can contribute to a sustainable social progress.

â¢ The aim with KTHs education for third-cycle studies is that the doctoral students should become independent, excellent researchers. The research (third-cycle) students should, after completed studies, be able to:

â¢ describe and explain theories and empirical results in the current field

â¢ formulate concrete research questions in the current field

â¢ use scientific methods and provide new knowledge through their own scientific studies

â¢ analyse and evaluate applied methods and results critically from own and others’ scientific studies

â¢
present and discuss research results within the scientific community

- present research in an educational way outside the science community and in 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

**The doctoral programme’s size and recruitment**

4.1 Expected number of registered students.

During the six-year period 2004-2009 was admitted on an average ten paragraphs doctoral students to the specialisation Theoretical Chemistry in the third-cycle subject area Biotechnology, the equivalent about. 40 at the same time active. It can be expected that a larger number of doctoral students will be admitted each year to the planned Doctoral program in Theoretical Chemistry and biology since the contents of "biology" are reinforced in the name of the new programme and therefore is expected reach out to a larger recruitment base. However, the number of admitted doctoral students will be continued depending on it the financial situation (size of faculty resources and external direct government fundings) as well as available supervisor resources.

4.2 Target groups

The target groups for Doctoral program in Theoretical chemistry and biology is students with degrees from Swedish or international higher education, typically Master of Science-program, in fields as chemistry, physics, biotechnology or mathematics. A special target group is students with background in mathematics and numerical analysis with interest in biological-/chemical-/material science-applications.

4.3 Entry requirements.

Entry requirements to Doctoral program in Biotechnology include partly a general entry requirements for postgraduate studies described in The Higher Education Ordinance, chapter 7, section 39:

General entry requirements have according to the Higher Education Ordinance chapter 7 section 39 the one that has:

1. been awarded a second-cycle qualification,
2. completed course requirements of at least 240 credits, of which at least 60 credits on
advanced level, or

3. In another way within or outside the country acquired equivalent knowledge.

Faculty board may for an individual applicant admit exception from the requirement on
genral entry requirements, if special circumstances apply.

For entry requirements to Doctoral program in Theoretical Chemistry and biology, the above described should
the bachelor-level or the advanced courses be in relevant subject area.

As supplements to these requirements can also so called
specific entry requirements exist for specialized areas.

These are described in the document "Study plan for the third-cycle subject area Theoretical Chemistry and
biology" (see appendix 1). Such specific entry requirements are assessed correspond to skills necessary to
be able to profit by the education and can for example involve knowledge/skills from
higher education in special fields of importance to the subject area or linguistic knowledge. The same
specific entry requirements apply to students with Degree of Doctor or Degree of Licentiate as aim.

4.4 Routines for recruitment, assessment of qualifications, and admission of doctoral students.
Recruitment, assessment of qualifications and admission of doctoral students will be carried out in
accordance with KTHs instructions. In case these instructions are changed such new instructions
shall apply to Doctoral program. For current version, KTHs regulatory framework should be visited.

For current admission regulations, see:
http://intra.kth.se/regelverk/utbildning-forskning/forskarutbildning/antagning/antagningsordning-forutbildning-
pa-forskarniva-vid-kth-1.27236

A financial plan for the initial two the years of the third-cycle courses and study programmes should be enclosed other
documents in
relationship with application for admission to postgraduate studies.

4.5 Available supervisors.
At the time (the autumn 2010) are four professors, two visiting professors and three docents/senior researchers
(with Degree of Doctor) the field of active in it Doctoral program as well as that one lectureship is currently being
appointed. Three professors at other schools on KTH will also participate in the programme (see appendix
2). Thus comes in total 13 paragraphs senior researchers (of which ten at the school for Biotechnology) are able to be appointed as principal supervisor in Doctoral program in Theoretical Chemistry and biology. Furthermore be it is expected that other senior researchers that are active in the section for Theoretical Chemistry today (and biology) in The school for Biotechnology will be promoted to docents in 5-10 years within the School for biotechnology, which makes that these are also expected to be able to be appointed as principal supervisor for doctoral students with licentiate or Degree of Doctor as aim. For current competence requirements on supervisor, see:

http://intra.kth.se/regelverk/utbildning-forskning/forskarutbildning/handledningstudieuppföljning/handledare-och-handledning-av-doktorand-1.27238

4.5 Available supervisors.

**Funding**

5.1 Funding of key persons in the programme.

The programme co-ordinator will become partly financed by the School for Biotechnology, KTH (equivalent about 20 % of a full-time employment). Principal supervisor and responsible, including the people who are included in the board for the programme will be financed via both faculty resources and external direct government fundings.

5.2 Funding of doctoral students.

Admitted doctoral students are expected to become financed mainly via external direct government fundings from different national and international sources including Vetenskapsrådet (VR), THE SWEDISH AGENCY FOR INNOVATION SYSTEMS, EU and China Scholarship Council, CSC) as well as industries and other private financiers (e.g Knot and the foundation of ALice Wallenberg and the Wenner-Grens foundation). Apart from these sources have the School for Biotechnology then 2008 an internal programme for appointment of so called Excellensdoktorander, with a background from KTHs Biotechnology program. Selected students are assigned a four-year grant from the school to be used for funding of a doctoral studentship under the guidance of a principal supervisor employed at the school for Biotechnology. Currently, 2-4 students been chosen a year, which freely can turn to which principal supervisor as preferably at the school. The plan is to continue with this programme also after the introduction of the Doctoral program at the School for Biotechnology (Biotechnology,
respective Theoretical Chemistry and Biology).

6. Courses

A Degree of Doctor of 240 credits (credits) contains a course module on 60 credits and a thesis component of 180 credits. Of the 60 credits that consist of courses should 60 % (= 36 credits) be courses on graduate level. A Degree of Licentiate of 120 credits (credits) contains a course module on 30 credits and an thesis of 90 credits. Of the 30 credits that consist of courses should 50 % (= 15 credits) be courses on graduate level. Third-cycle courses that are given by KTH are divided into four classes:

(A) Advanced courses

(B) Skill courses

(C) Broadening courses

(D) Other courses

The Doctoral program in Theoretical Chemistry and biology include only a third-cycle subject area, Theoretical chemistry and biology, except for some underlying specialisations.

For this third-cycle subject area, a course block has been compiled, containing compulsory courses (O) and recommended courses (R) from the different course classes (A-D) (see appendix 3). Compulsory courses should be given at least every second year. Some courses are compulsory for all specialisations, and constitutes thereby joint courses for Doctoral program in Theoretical Chemistry and biology. The total number credits that are constituted by compulsory courses vary between 16.0 and 36.5 credits, depending on degree (licentiate or Degree of Doctor) and other conditions. Possibility to substitute a compulsory course with a comparable course should be after assessment at programme co-ordinator and co-ordinator for doctoral education.

It will be arranged regularly literature seminars (extending over a whole year) where broader issues of more general and general nature are brought up and are discussed in plenary meeting with intention to expand competence. It will be compulsory to participate in at least a such whole-year course.

7. Description of the systematic quality assurance procedures

The aim for the systematic quality assurance procedures is to ensure that the general aims with the third-cycle courses and study programmes is satisfied.

7.1 Steering group for the programme.

A steering committee for the Doctoral program should be shaped where
programme co-ordinator, co-ordinator for doctoral studies, two to three principal supervisors, and a doctoral student should be included and that in regularly held meetings (about two meetings a year) should discuss quality aspects concerning specific components in the process, including:

- the recruitment process
- the supervisors's skills
- course and seminar activities, including documented evaluations
- the quality of theses
- student completion rates
- employability after examination

7.2 Supervisor's forum

The supervisors in a certain specialisation, or in a group of specialisations, be recommended to be met at least once each year to discuss and exchange experiences about the doctoral program, the courses, the quality of the research, questions about supervision and the progress of the doctoral students.

7.3 Evaluation of the quality of courses and theses.

All courses should be subject to written evaluation.

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-forforhandsgranskning-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 imply that these criteria not be considered applicable or relevant, should be discussed with the co-ordinator for doctoral studies and the Dean at the School for Biotechnology, KTH.

Doctoral thesis

Compilation thesis

The thesis should normally be based on four articles.

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

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

â€“ The doctoral student should emerge as "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".

â€“ For all of the included articles should the own contribution of doctoral students be significant and clearly stated.

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

â€“ In those cases where a thesis is only based on manuscripts that not have been published still or been 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, as well as the examining committee.

Monograph

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

â€“ The thesis should previewed before printing of at least two senior researchers, the principal supervisor as well as the co-ordinator for doctoral studies.

Licentiate thesis

Compilation thesis

â€“ The thesis should normally be based on two articles.

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

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

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

â€“ For all of the included articles should the own contribution of doctoral students be significant and clearly stated.

â€“ 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 of at least one senior researcher as well as the principal supervisor.

â¢ If the thesis does not contain some 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.

Monograph

â¢ Monographs should be avoided. KTH has a stated ambition that the contents of theses should be publishable in international referent-granskade ("peer reviewed") scientific magazines.

â¢ The thesis should be previewed before printing of at least two senior researchers, the principal supervisor, as well as co-ordinator for doctoral studies.

7.4 Infrastructure available for doctoral students in the doctoral program.

At KTH, a very resource-rich new center, CSE- Swedish E-science Research centre (SERC) has been created as a result of a governmental strategic research initiative. SERC takes a national responsibility in E-science as host for the large majority of Swedish E-science infrastructure through national computation centers where parallel computing (PDC) at KTH takes a leading role. The recent initiative by KTH to act as host for an European PRACE-system on parallel-computing for peta-flop-calculations is also highly relevant, as it will give doctoral students in the programme availability to a resource with world-leading technology in terms of both hardware and software. The purchase of a 300 Tflop CRAY-dator, in full operation from January 2010, places KTH in a leading position as regards simulation capacity. The section has access to a large part of the resources at SNIC (Swedish National Infrastructure) at national data centers and has access to large resources of international computational power, e.g. in China through KTH-USTC-center that is led by the section for Theoretical Chemistry (and biology). All initiatives and resources will be directly connected to the implementation of Doctoral program. As regards other sections in the School for Biotechnology, KTH are two facilities for laboratory work; AlbaNova Universitetscenter as well as parts of the so called Science left Life-laboratoriet that is located at Karolinska Science Park, next to Karolinska Institutet (Solna). Both these laboratories represent modern environments that are adequately equipped for experimental activities in life science, involving handling, storing and
disposal of biological material (fume-hoods, incubation rooms, fridges, freezers, autoclaves, etc). Furthermore, the instrumental standard is relatively high; as example can be mentioned instrumentation for (in) measurements of biomolecular recognition (biosensors, flow cytometers), (ii) efficient sequencing of nucleic acids (DNA-sequencing), (iii) production and scanning of biopolymers (nucleic acids and proteins), (iv) DNA-amplification (PCR-instrument), (v) spectrophotometers, (vi) centrifugation of biological material, (vii) bioseparation (chromatography), (viii) mass-measurements (mass spectrometry), (ix) fermentation with cell culture in different scales (2 to 500 litres).

All doctoral students are assigned a desk with a computer and access to the normal office supplies (printer, fax, scanner, telephone, etc). The pantry area is for preparation of personal food.

The school for Biotechnology, KTH provide normal administrative service to doctoral students, that handling of salary, insurances, holiday, parental leave, etc A department for handling of personnel issues (HR-department) are also available. KTHs large central library is available for all students. Doctoral education questions that concern the School for Biotechnology is handled of both local and more central departments:

- Programme co-ordinator
- Staff at Chemistry-, Chemical engineering-, and Biotechnology-offices (KKB)
- Local doctoral education administrators
- Director of doctoral education

Courses

The courses within the doctoral programme are all offered within a third-cycle subject and are therefore presented in the study plan for the subject.

Quality enhancement activities

National and international network

International networks

The section for Theoretical Chemistry (and biology) coordinates or participates in a large number of networks at the local, national and international level (see appendix 4). The section has a salient international profile at the doctoral students (35 of the today 40 enrolled the students are from the abroad), and has a long successful history of funding via Swedish funding agencies as SI, The Swedish International Development Authority, KVA and through funding agencies from the students’ own countries of registration as CAPEC and CNPq in
Brazil, China Scholarship Council, Indian Institute of Science and through different European programmes (especially Marie Curie) that the section have coordinated and participated in. It is also strong nordic network including participation in a Nordic Network of Centre of Excellence, with exchange of students and seniors and in a Masters Educational programme that includes five nordic universities (start the autumn 2011). The section also constitutes a main partner in the Scandinavian DALTON-project, with the associated data simulation programs that are necessary for many course assignments. DALTON has more than 2000 licenses for our Doctoral program and will continuously equip new students as well as alumni with cutting edge software in molecular/multi-scale modeling. Yet another valuable strategic access for the students is they strong bands that been built with a large number international groups in Japan the USA and Europe and in particular with emerging nations such as China, India and Brazil. Only with China is there an exchange of students and of science, with 14 leading universities including co-administration of a KTH-China research center (KTH-USTC Centre in Bio and Nanomaterial). With India there are five externally financed programmes including a tri-lateral KTH-Indien-Kina research centre. These networks constitute a basis for recruitment at all levels including doctoral students, and for career possibilities for students after the degree.

Industry connections.

Existing industry connections and support for the section will be healthy for the programme, e.g. contacts with AstraZeneca, ACREO, Portendo LTD, Biovitrum LTD, Biotage LTD and LightLab Sweden LTD. Meetings will be arranged where researchers from the industry in computer science are invited. These meetings that also involve KTH alumni in computer science can contribute with career information for the students of the Doctoral program. The meetings are arranged as series of lectures from industry representatives, where the role of the computer science is discussed including how cooperation with and recruitment from academia takes place. Group discussions are held, where students are given a possibility to interview industry representatives and learn more about application fields that can be current for their careers.

Local level.

In the above-mentioned SERC-center, the department is responsible for âthe electronic structure community ", together with KTH Materials Science (Anna Delin). The department is active within
a recently started EU programme “SCALALIFE” (Scalable Software Services left Life Science, coordinated by PDC), together with engineers at PDC for software development as well as KTH Theoretical Physics (recently appointed professor Erik Lindahl) which will develop multiscale software (Quantum-Classical) for life-science applications and with full adaptability to modern multi-core hardware (e.g. through the European PetaFlop PRACE-project). Furthermore, the department is a founding member of the KTH Computer Centre and Engineering (KCSE), that involves seven KTH institutions. This centre will, at the beginning of 2011, be incorporated into SERC but will maintain its cross-border Doctoral program in computer simulation, where the section is responsible for several courses. There will thus be strong synergies with this programme during the three years of activities that remains. The department coordinates a NORDIA-financed Nordic Summer School for doctoral students in ”Multiscale Modelling and Simulation in Science”, that is carried out twice a year (three-week course) at AlbaNova Universitetscenter. In supplement to formal (contractual) networks and regularly recurrent exchange programmes with international universities that are associated with the programme, admitted students are encouraged to visit other research teams and laboratories for different length periods to learn a new technology/methodology or to carry out joint experiments. Larger EU-projects and research ”centers” constitute excellent environments for network building between academic researchers and between academic researchers and industry.

The above is enumerated and defined in appendix 3.

Further instructions for registration

Appendixes

Appendix 1: Study plan for third-cycle subject Theoretical Chemistry and Biology (TKOB).

Appendix 2: List containing names and subject areas of supervisors within the programme

Appendix 3: Presentation of the programme’s national and international network
Doctoral programme — Theoretical Chemistry and Biology

Appendix 1: Study plan for third-cycle subject Theoretical Chemistry and Biology (TKOB).

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-Årars-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

L:
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

D:
Skill courses

Theoretical Chemistry and biology
BB3110 Programming 5 R
IN5113 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
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

â€¢ The thesis should normally be based on four articles.

â€¢ 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.

â€¢ 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”.

â€¢ For all of the included articles should the doctoral student’s own contribution be significant and clearly indentifiable.

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

â€¢ 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

â€¢ Monographs should be avoided. KTH has a stated ambition that the contents of theses should be published in international refereed (“peer reviewed”) scientific magazines.

â€¢ 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

â€¢ The thesis should normally be based on two articles.

â€¢ 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.

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

â€¢ For all of the included articles should the doctoral student’s own contribution be significant and clearly indentifiable.

â€¢ 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.
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.

Monograph

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.se). 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.
Doctoral programme — Theoretical Chemistry and Biology

Appendix 2: List containing names and subject areas of supervisors within the programme

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

Prof His Ågren
Prof Faris Gelmukhanov
Prof Yi Luo
Prof Olav Vahtras
UnivL MÅyrten Ahlquist
UnivL Zilvinas Rinkevicius
Doctoral programme — Theoretical Chemistry and Biology

Appendix 3: Presentation of the programme’s national and international network

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