Programme syllabus

Master's Programme, Computational Chemistry and Computational Physics, 120 credits
Masterprogram, beräkningskemi och beräkningsfysik
120.0 credits

Valid for students admitted to the education from autumn 14 (HT - Autumn term; VT - Spring term).

This is a translation of the Swedish, legally binding, programme syllabus.

Programme objectives

A Master in Computational Chemistry and Physics should:

- Have good ability to describe and apply various mathematical models to solve the chemical and physical problems.
- Have a good understanding of methods and programming languages for scientific programming.
- Formulate and approach new problems in molecular computational science in a scientific way.

Knowledge and understanding

A Master in Computational Chemistry and Computational Physics should be able to:

- Solve real chemical, biological and physical problems using the methods taught in the master's program. The student should be able to determine which method is most suitable for solving the specific problems.
- Plan a simple research project by identifying the problem and methodology by which the problem can be solved.
- Write simple software for use in scientific programming.
- Work in international environments.
- Work effectively in groups.
- Present and communicate results and skills in both written and spoken English.

Skills and abilities

A Master in Computational Chemistry and Computational Physics should be able to:
• Critically examine a problem and in an independent way to obtain information and knowledge that is necessary to have a qualified opinion.
• Formulate and approach new problems in molecular computational science in a scientific manner.
• Identify the need for new knowledge in the study and take responsibility for keeping their own knowledge current.

Ability to make judgements and adopt a standpoint

Extent and content of the programme

*Computational Chemistry and Physics* is a two-year (120 credits) master programme, second cycle, including a Degree Project, advanced level, 30 credits.
Project: Specialization in Chemistry and Physics (KTH).
The instruction language is entirely English.

Specializations within the program

• **University of Tromsø (UIT):**
  Ab initio method development, relativistic effects, reactions to solvent, molecular characteristics, biomolecular modeling, wavelets.

• **Royal Institute of Technology (KTH):** Biotechnology and chemistry including biomolecular modeling, multi-scale modeling, molecular biotechnology, organic and enzymatic catalysis.

• **University of Iceland (HI):**
  Reaction rates, dynamics, density functional theory, periodic table, solid state chemistry / physics.

• **Helsinki University (HU):**
  Development of methods for electronic and nuclear degrees of freedom, periodic, multi-scale modeling, nano-systems, materials, processes not in equilibrium. optical and magnetic properties of molecules, biomolecular modeling, finite element methods.

• **Göteborg University (GU):**
  Reaction dynamics, calculations of spectroscopic properties.

Programme structure linked to programme goals and degree objectives.
In order to ensure that students achieve the objectives specific to this programme and the general objectives of the master of science degree at KTH, each student's curriculum must be developed in consultation with the programme director.

During study year 1 the programme consists of the following mandatory courses:
*Computational Chemistry*
*Molecular Modeling*
*Mathematical and numerical methods (GU)*
*Scientific Programming (HU)*
as well as the following courses:
*Photonics*
*Multiscale modeling*
During study year 2 the programme consists of the following mandatory courses:

- *Theory and Methodology of Science with Applications*
- *Degree Project, advanced level*

as well as the following course:

- *Enzymatic and Organic Catalysis*

### Eligibility and selection

In order to be eligible to apply to the master’s programme, a relevant higher education degree of at least 180 credits, degree of bachelor in science or in engineering, preferably in chemistry, chemical engineering, technical physics, applied mathematics or computational science is required. Other corresponding technical or natural scientific degree on the first level can also give eligibility, provided that basic courses in mathematics, computer science, as well as chemistry and/or physics are included. Other studies or work experience are judged on the basis of the actual competences which are referred to.

A sound and documented knowledge of written and spoken English - equivalent to a minimum TOEFL written test grade 4 or IELTS score of 5.0 for non-native speakers - is required from all applicants outside of the Nordic countries.

The following (KTH) directives will be followed:

- Paper-based test: total result of 550 (written test, grade 4)
- Internet-based test: total result of 79 (written test, grade 7)
- Computer-based test: total result of 213 (easy rating, grade 4)

Only academic training is accepted.

The selection to the programme is based on an evaluation of the following criteria:

- University/higher education institute, courses relevance for the program, grades, letter of motivation, recommendation letters and references.

All applications will be received and handled by the University of Tromsø admission office, though the letters of acceptance to the program will be sent out by the host universities at which the student is accepted.

### Implementation of the education

#### Structure of the education

The studies start with a common semester with two mandatory courses, *Computational Chemistry* and *Molecular Modeling*, offered by each individual partner, as well as two mandatory courses, *Mathematical and Numerical Methods for Chemists*, offered by Göteborg University (GU) and *Scientific Programming* by Helsinki University (HU).

The student needs to select an additional set of 30-60 credits in optional courses offered by the participating Universities. In addition, the student will have to complete a Degree project, advanced level, 30 credits. It is a goal for the programme that the students are supervised by senior researchers from at
least two different host institutions, and that extended stays at a different host institution is part of the study programme (a minimum of three months at a different university than the home university of the student).

All students must also complete the course *Theory and Methodology of Science with Applications* (7.5 credits) during the second year of studies. Since this course is limited to 7.5 credits, while the other course within the programme are all 10 credits (Degree project, 30 credits), this should be supplemented by a suitable course so that students reach the goal of 120 credits required for the masters degree. A recommended course is *Information Search*, 3 credits since this course would prepare the student to seek information effectively for the degree project.

The academic year of the higher education programs at the different partner universities consists of about 40 weeks divided into either 2 or 4 periods. Information about the academic year at the different partner universities is available on the local home pages.

**Structure of the education**

The programme is given in the form of courses. The courses which are given in the programme can be found in Appendix 1.

The student register for the individual courses in the way that each one of their partner Universities decides. For all courses provided, there exists local course codes to facilitate the acknowledgment of the course content, even though the actual course is conducted by a different host institution, where the student follow the course, either on site or through e-learning activities. At KTH the foreign courses will be registered as credit transfer, and will not be assigned a KTH course code.

For students accepted at KTH, it is mandatory to follow the course *Theory and methodology of science with Applications*.

**Courses**

The programme is course-based. Lists of courses are included in appendix 1.

*Courses given by KTH:*

Computational Chemistry with Project (Corresponding to “Molecular Quantum Mechanics” at the Nordic level).

Molecular Modeling with Project (Corresponding to “Atomic Scale Simulations” at the Nordic level).

Computational Nanotechnology and Bio Nanotechnology

Enzymatic and Organic Catalysis

Multiscale modeling in Chemistry and Biology

*Courses given by the partner universities:*

MC3: Mathematical and Numerical Methods for Chemists (GU)
MC4: Scientific programming (HU)

OC1: Rates of transitions and long time scale evolution (HI)

OC2: Transport through molecules and nanostructures (HI)

OC3: Chemical Kinetics and Dynamics (GU)

OC4: Quantum Chemical Methods (UIT)

OC5: Relativistic Quantum Chemistry (UIT)

OC6: Molecular Properties (UIT)

OC7: Theory and Computations of Nanosystems (HU)

**Grading system**

Courses in the first and the second cycle are graded on a scale from A to F. A-E are passing grades, A is the highest grade. The grades pass (P) and fail (F) are used for courses under certain circumstances.

The different partners grade courses according to different grading scales.

- At the Universities of Tromsø and Helsinki and at KTH, courses are graded on a scale from A - F, A-E are passing grades, A being the highest grade. In certain cases, courses may be graded as pass (P) or fail (F).
- At the University of Iceland, courses are graded on a scale from 0 to 10, 5-10 are passing grades, 10 being the highest grade
- At Göteborg University courses are graded on the scale *Pass with distinction, Pass and Fail* (*Väl godkänd, Godkänd and Underkänd*)

**Conditions for participation in the programme**

A student accepted to the programme is required to, before November 15 of the first semester, submit a plan for the last three semesters of his/her study programme, detailing the courses which he/she intends to take and in which semester, as well as a description research project 30 credits, a title and a project description for the research project as well as naming at least two supervisors that are not from the same host institution. The programme committee evaluates the study programme and may suggest changes in order to optimize when courses are being offered. Once accepted by the programme committee, this study plan will form the foundation for the expected study progress of the student.

A student who fails to follow the accepted study plan must consult with the programme director. Adjustments to the individual study plan may then be made. The main goal with these changes to the study plan is that the student should complete remaining courses/course-parts during the next study year.

In the study plan, the remaining courses/course-parts and also suitable courses from the next study year are included. Special regard is taken to the prerequisites of the courses yet to be taken.

**Recognition of previous academic studies**
Under certain circumstances, and in agreement with the programme committee, credits for previous studies in the Nordic countries or abroad can be received according to the local policy of KTH. Students wishing recognition of previous academic studies must submit an application to the Programme committee

For more information see:

Studies abroad

Each student is assigned a home university where he/she will be resident. This choice is dependent on the optional courses he/she chooses. Two of the common courses (MC3 and MC4) will be conducted by web based E-learning. The two Icelandic courses are planned to be given through summer internship at Iceland.

Student exchange between the other Nordic countries will be determined on a case to case basis. However, every student is required to spend at least three months at one of the partner universities. Experience from previous exchange of PhD students between the partners of this programme have been very good.

Degree project

To start the degree project, advanced level, 30 credits, at least 50 credits within the programme should have been achieved, all compulsory assignments should have been attempted and at least 90% of these assignments should have been passed.

In order to fulfil requirements for obtaining a masters degree, the project must be part of the required in-depth studies at second level in the main field of study for the programme. The topic of the project must be accepted by the programme committee.

The project can be performed at any of the partner universities.

The project thesis will be graded according to the grading scale used at the host institution of the Master student.

Degree

Master of Science, Master (120 credits) is obtained after completion of the programme. This will be a joint degree involving the different partner institutions, though for some of the partners, a dual degree may have to be offered in a transitional phase. The degree is issued by the host institution at which the student was accepted in the programme, which is based on his/her selection of host institution when applying for the programme.

The individual study plan must be designed so that students, when they graduate, have fulfilled the requirements for this joint degree and have completed courses comprising 120 credits of which:

"At least 90 credits are at the second level, of which at least 60 credits (including a degree project, advanced level, at least 30 credits) with in-depth studies in the main field of study."
This degree is called Master of computational chemistry and physics. The text on the degree certificate states the name of the educational programme completed by the student beside the main field of study.

When all courses needed are completed and reported, the student must personally apply for a degree certificate. This is done by filling in (the upper part of) the application form accompanied by an attested photocopy of previous University degree (B.Sc. or a B.Eng., or equivalent).

Appendix 1 - Course list
Appendix 2 - Programme syllabus descriptions
Appendix 1: Course list

Master's Programme, Computational Chemistry and Computational Physics, 120 credits (TBKFM), Programme syllabus for studies starting in autumn 2014

General courses

Year 1

Mandatory courses (20.0 Credits)

<table>
<thead>
<tr>
<th>Course code</th>
<th>Course name</th>
<th>Credits</th>
<th>Edu. level</th>
</tr>
</thead>
<tbody>
<tr>
<td>BB2280</td>
<td>Molecular Modeling</td>
<td>7.5 hp</td>
<td>Second cycle</td>
</tr>
<tr>
<td>BB2285</td>
<td>Project in Molecular Modelling</td>
<td>5.0 hp</td>
<td>Second cycle</td>
</tr>
<tr>
<td>BB2300</td>
<td>Computational Chemistry</td>
<td>7.5 hp</td>
<td>Second cycle</td>
</tr>
</tbody>
</table>

Supplementary information

During study year 1 the programme consists of mandatory courses at KTH (see list) and mandatory distance courses

- Mathematical and numerical methods (GU)
- Scientific Programming (HU)

as well as the following two new courses

- Photonics
- Multiscale modeling

Year 2

Mandatory courses (7.5 Credits)

<table>
<thead>
<tr>
<th>Course code</th>
<th>Course name</th>
<th>Credits</th>
<th>Edu. level</th>
</tr>
</thead>
<tbody>
<tr>
<td>AK2036</td>
<td>Theory and Methodology of Science with Applications</td>
<td>7.5 hp</td>
<td>Second cycle</td>
</tr>
<tr>
<td></td>
<td>(Natural and Technological Science)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Appendix 2: Specialisations

Master's Programme, Computational Chemistry and Computational Physics, 120 credits (TBKFM), Programme syllabus for studies starting in autumn 2014

This programme has no specialisations.