UiT The Arctic University of Norway

PROGRAMME DESCRIPTION

Computational Chemistry - master

120 credits

Tromsø

The program description has been approved by the Faculty of Science and Technology 03.09.2025.

Study program name	Computational Chemistry - master
Degree obtained	Master of Science in Computational Chemistry
Target group	The Master's programme in Computational Chemistry is designed for students with a strong interest in using theoretical and computational approaches to solve problems in chemistry and related scientific disciplines. This programme is particularly relevant for those who wish to gain deep insight into the structure, properties, and reactivity of molecules through modelling and simulations, and who aim to contribute to fundamental research, technological innovation, or the development of sustainable solutions in chemistry. The programme targets students holding a bachelor's degree in chemistry, molecular sciences, physics, mathematics, or informatics, with sufficient background in chemistry. It is well suited for individuals seeking careers in academia, research institutes, or industries where computational modelling, quantum chemistry, and molecular simulation play a central role — such as in pharmaceuticals, materials science, catalysis, biotechnology, or environmental technology. Students who are motivated to develop programming skills and apply high-performance computing to understand molecular systems will find this programme particularly rewarding. The programme also offers a solid foundation for further doctoral studies in theoretical and computational chemistry or related fields.
Admission requirements, required prerequisite, recommended prerequisite knowledge	The student is eligible according to UiT - The Arctic University of Norway's general admission rules: • General admission requirements - Master. • A bachelor's degree (180 ECTS credits) in one of the natural sciences; Chemistry, Molecular Sciences, Mathematics, Physics, Informatics OR an equivalent degree following a programme of study of minimum 3 years (More information on bachelor's degree requirements) • The bachelor's degree must contain a minimum of 30 ECTS in chemistry courses on bachelor level, and a minimum of 80 ECTS (or equivalent) specific to our master discipline • Applicants must have a minimum grade average comparable to a Norwegian “C” (3.0) in the ECTS scale, see the UiT webpage for international admissions for more information on how the point average is calculated.

	• International students from non-Nordic countries (except students with English as their mother tongue), must meet the Department of Chemistry's English proficiency with a recommended minimum score of 6.5 on each part of the IELTS test, minimum scores of 22, 22, 22 and 25 (reading, listening, speaking and writing, respectively) on the TOEFL test, C1 Advanced or C2 Proficiency level on Cambridge ESOL Examinations, or minimum C1 level on The European language certificate (telc)
The study program's learning outcome	**Knowledge** The candidate… • has advanced knowledge of theoretical chemistry and the underlying principles of quantum mechanics and molecular modelling • has in-depth understanding of modern methods used in computational chemistry, including wavefunction theory, density functional theory, and molecular mechanics • is familiar with state-of-the-art software, algorithms, and computational strategies for modelling chemical systems • has knowledge of how computational chemistry contributes to analysis and innovation in areas such as catalysis, drug discovery, spectroscopy, and materials science • has insight into the role of high-performance computing in enabling advanced analysis in chemical research **Skills** The candidate… • can independently select and apply appropriate computational methods to analyse molecular structure, properties, reactivity, and dynamics • can perform quantum chemical and molecular simulations using modern computational tools • can critically assess computational results and evaluate convergence, accuracy, and reliability of the data • can interpret and explain the outcomes of simulations in terms of chemical theory and experimental relevance • can write reproducible scripts, manage simulations on local and high-performance computing platforms, and automate workflows • can carry out limited research projects in computational chemistry under supervision, and document findings in accordance with research ethical standards

	General competence The candidate… • can communicate scientific ideas, problems, and solutions clearly in oral and written forms • can critically analyse scientific literature and integrate knowledge from multiple sources to solve complex chemical problems • can analyse and evaluate and reflect on the environmental, ethical, and societal implications of computational work in chemistry • can contribute to interdisciplinary collaborations and apply computational chemistry in broader contexts such as sustainable development and technological innovation
Academic content and description of the study program	The Master's programme in Computational Chemistry provides advanced knowledge and skills in the theoretical description and computational modelling of molecular systems. This is a full-time and campus-based programme focusing on modern quantum chemical methods, molecular mechanics, and numerical modelling to investigate molecular structure, bonding, properties, dynamics, and reactivity. The curriculum includes core topics such as wavefunction theory, density functional theory (DFT), statistical thermodynamics, and spectroscopic simulation. Students are trained in the use of scientific software and high-performance computing infrastructure, as well as scripting and protocol development to automate calculations and analyse results. Teaching is closely integrated with research activities, ensuring that students are exposed to current challenges and innovations in the field. Typical applications of computational chemistry introduced in the programme include: • Reaction mechanism modelling and transition state analysis • Spectroscopic property predictions and structure elucidation • Enzyme function, ligand binding and rational drug design • Materials and catalyst modelling, including nanostructures and surfaces • Development and benchmarking of quantum chemical methods Throughout the programme, students will strengthen their understanding of how theoretical models relate to experimental observables and will learn how to critically assess the reliability of computational predictions. Students may specialise in method development or applications within fields such as organic chemistry, biochemistry, environmental chemistry, or materials science. The programme consists of 120 ECTS credits over two years, including a 60 ECTS master's thesis based on independent research. All teaching and supervision are conducted in English. Students will become part of the Theoretical and Computational Chemistry research group at the Department of Chemistry, and benefit from access to national and international scientific computing resources.

Program outline

The Master's degree program in Computational Chemistry at UiT has a duration of 2 years and equals a total of 120 ECTS (Table 2). Each Master's candidate works on a research project to complete an independent scientific dissertation (thesis, 60 ECTS) under supervision. In addition, the programme includes topical coursework, where 40 ECTS are obligatory for all students admitted to the program, and 20 ECTS are to expand on the students chosen discipline and other special curricula (total 60 ECTS).

Table 2 Outline for the Master's degree program in Computational Chemistry.

Sem	Computational Chemistry		
1st	KJE-3502 Biomolecular structure and modeling	KJE-3101 Quantum chemistry	BED-3200 Bærekraftig innovasjon
2nd	KJE-3102 Computational chemistry	KJE-3503 Computational material science/ Optional course	Thesis
3rd	Special curriculum/ Optional course	Thesis	
4th	Thesis		

Optional courses should be chosen from the list below (Table 3) and from other relevant master level courses at UiT or other institutions. Courses not on the list must be approved in advance by the Department of Chemistry.

Table 3 List of optional master level courses at the Department of Chemistry

KJE-3103$	Quantum chemical methods
KJE-3104$	Relativistic quantum chemistry
KJE-3201$	Bioinorganic chemistry
KJE-3317	Applied spectroscopical analysis (spring)
KJE-3316$	Radiopharmaceutical chemistry
KJE-3805/ 3810/3820	Individual special curriculum – Master's degree (5/10/20 ECTS)

$ Course given at irregular intervals

Learning activities, examination and assessment

Courses are taught as classes or as individual curriculum. Various assessment methods are applied. Courses are assessed through oral or written exams, some through assessment of a laboratory or project report, and some as a combination of methods. Up-to-date course descriptions are available online.

The study program's relevance	Computational chemistry plays a central role in modern chemical research, development, and innovation. The Master's programme in Computational Chemistry equips students with theoretical insight and practical skills to model, predict, and analyse chemical systems using state-of-the-art computational methods. Graduates are qualified for a wide range of careers in academia, research institutes, and industry where simulation and modelling are essential tools — such as in the pharmaceutical, chemical, materials, and energy sectors. They may contribute to the development of new drugs, catalysts, and functional materials, or help optimise industrial processes by providing molecular-level understanding and predictions. The programme also provides a strong foundation for doctoral studies in theoretical and computational chemistry or related disciplines, including chemical physics, materials science, and molecular biosciences. Due to the increasing importance of data-driven approaches and digitalisation in the natural sciences, graduates are also well suited for positions in high-performance computing, scientific programming, and data analysis. The relevance of the program is further strengthened through close integration with active research groups and access to national and international scientific computing infrastructure. Students work on real research problems and gain experience in collaborative scientific environments, preparing them for further academic training or professional careers in both research-intensive and applied contexts.
Work scope	As a Master´s student you become a member of the research group in Theoretical and Computational Chemistry at the Department, with an assigned thesis supervisor. You are advised to contact potential supervisors already in the first semester in order to start planning course work and the research project, which may be started in the first year. Throughout the research project, you may work closely in teams with doctoral students, post-doctoral fellows and senior scientists, and for some projects, local industry and enterprises. To achieve the learning outcomes of the programme, students are expected to work on average at least 40 hours per week throughout the year on project and courses, including lectures, lab and seminars.
For master's theses/independent work in master's degrees	The Master´s thesis (60 ECTS) must be an independent scientific dissertation, completed under the supervision of a scientific staff member or a postdoctoral fellow affiliated to Department of Chemistry, UiT.
Language of instruction and examination	The language of instruction and examination is English, and all syllabus material is in English. The Master´s thesis must be written in English.

Student exchange	The Master´s program is structured such that the student can spend periods of their study abroad, preferably in the third semester. Student exchange can be formal courses, or visits to other labs and institutions to learn new techniques. Formal exchange programs with international Universities exist, (see the study program's web pages for more information). However, visits abroad are generally arranged individually, depending on what is relevant for the Master´s project, and on the collaborations of the supervisor. Courses must be approved in advance.
Administrative responsibility and academic responsibility	Faculty of Science and Technology, Department of Chemistry
Quality assurance	The study programme and all courses are evaluated according to the University´s quality assurance system. Course evaluation consists of both student and teacher reports.
Other regulations	Utfyllende bestemmelser for toårig mastergrad (120 studiepoeng) ved Fakultet for naturvitenskap og teknologi Supplementary provisions for the two-year master's degree programme (120 credits) at the Faculty of Science and Technology