SOFIA UNIVERSITY "ST. KLIMENT OHRIDSKI"

FACULTY OF CHEMISTRY AND PHARMACY

CURRICULUM

Approved by: ....

Approved by the Academic Council with Record of Proceedings № ...6... / ...26 март 2025 г.

Professional Field: 4.2 Chemistry

Educational and Qualification Degree: Master of Science

Subject Area: Computer chemistry

C	H	C	2	5	2	4	2	5

Master programme: Computational chemistry – in English

Form of Study: full-time
Length of Study: 3 semesters

Professional Qualification: Master in Computer chemistry – Computational chemistry

Qualification Description

Subject Area: Computer chemistry
M. Sc. programme: Computational chemistry – in English

1. Aims and Educational objectives

The programme offers theoretical training in the area of: quantum chemical methods for description of atoms, molecules, and periodic systems; structure-activity and structure-property relationships; molecular mechanics and molecular dynamics; rational molecular design; prediction and analysis of spectral characteristics; study of the mechanisms of chemical processes at the molecular level. The educational objective is achieved by courses focused on presenting in detail the major theoretical methods and on elucidating the structure-composition-properties relationship of chemical compounds.

2. Description of the educational content (knowledge and skills required for a successful professional realization; general and theoretical background, specific areas of study, etc.)

The lectures of all courses are meant to provide theoretical training while the practical application will be mastered during the seminars by solving specific computational problems and/or performing molecular modelling within a particular chemistry-related assignment. The independent work of the students is stimulated – almost every course envisages individual student projects. The M.Sc. theses involve research on an up-to-date research topic and promote original scientific contributions.

3. Professional and general competences, specific competences

Training of specialists with a definite profile at the Master EQF level in the field of Computational chemistry is provided. The graduates should acquire specific practical skills for performing analysis of numerical data from specialized software packages and for using various scientific programming languages to develop their own codes.

4. Professional realization (according to the National Classification of Occupations in the Republic of Bulgaria /based on the International Standard Classification of Occupations (ISCO)/ and in reference to the place of the future specialists in the National Qualifications Framework for higher education and the European Qualifications Framework for higher education)

The graduate students with M.Sc. degree in Computer chemistry - Computational chemistry can continue their education in a related PhD programme or pursue successful career as researchers in computational modelling around the world. A business career is an equivalent option in industries like: ICT; pharmacy; biotechnologies; materials science; micro- and optoelectronics; photovoltaics; laser fabrication; ecology; nanotechnologies; catalysis, etc. The acquired skills allow also various occupations related to data management and data processing.

The graduates obtain competencies in field 2113 of the National classification of professions and positions in the Republic of Bulgaria (codes 6001 – 6030). They acquire competencies also from the following areas: 2511 Systems analysts, 2512 Software developers, 2514 Applied software developers, 2519 Developers of software and software applications and analysts, 2521 Designers and administrators of databases, 2529 Database and network specialists.

The graduates of the "Computational Chemistry" Master programme fall within level 7 of the European qualifications framework classification.

5. Admission requirements

The candidates should hold B.Sc. degree in Chemistry or in a related area of study (certified by official Bulgarian translation of the diploma). They will be graded by their average diploma score for admission.

C 2524
CHC252425

Area of Study "Computer Chemistry" / Master's Degree Program "Computational Chemistry - in English"

admission winter semester of 2025/2026 academic year

№	Course code	Course Title	Type – C, E, O	Semester	ECTS credits	Classes - total number: Total	Lectures	Seminars	Practical classes	Self study	Classes per week	Assessment* - e, ca, ce, cont.
1	2	3	4	5	6	7	8	9	10	11	12	13
Core courses												
1	C018	Quantum chemistry for molecular systems	C	1	8	240	60	-	45	135	7	e
2	C025	Quantitative structure-activity relationships of bioactive compounds	C	1	5	150	30	-	30	90	4	e
3	C036	Programming	C	1	6	180	30	-	45	105	5	e
4	C045	Molecular mechanics	C	1	5	150	30	-	30	90	4	e
5	C056	Term project	C	1	6	180	15	-	45	120	4	ca
6	C064	Modelling of periodic systems and nanostructures	C	2	4	120	30	-	30	60	4	e
7	C074	Hybrid (QM/MM) methods	C	2	4	120	30	-	30	60	4	e
8	C084	Computational methods in spectroscopy	C	2	4	120	30	30	0	60	4	e
9	C095	Molecular dynamics and Monte Carlo simulations	C	2	5	150	45	-	30	75	5	e
10	C109	Applied computational chemistry	C	2	9	270	30	-	105	135	9	ca
11	C115	Analysis, reference and presentation of theoretical studies	C	3	5	150	30	-	30	90	4	ca

The Faculty Council has decided that min. 50% of the total education load is independent study of the students

Type of grading:
e-exam, ca-current assesment,
m-matriculation,
a-advances to the next semester

Elective courses – *courses with minimum of 4 ECTS (total) need to be elected*														
1	E	0	1	4	Introduction to Linux shell programming and data processing	E	2	4	120	30	-	30	60	4	e
2	E	0	2	4	Molecular kinetics and thermodynamics by ab initio MO calculations	E	2	4	120	30	-	30	60	4	e
3	E	0	3	4	Molecular modeling of excited states	E	2	4	120	30	-	30	60	4	e

**Students are allowed to elect also other courses from all M.Sc. programs at the Faculty of Chemsitry and Pharmacy, Faculty of Physics, Faculty of Biology, Faculty of Matehmatics and Informatics, Faculty of Economics and Business Administration, Faculty of Classical and Modern Philology , Faculty of Slavic Studies, Faculty of Pedagogy, Faculty of Educational Studies and the Arts, Faculty of Geology anf Geography, Faculty of Philisophy, Faculty of Hystory.*

***Courses with successfully passed exams during a period of academic mobility at a foreign higher education institution in the framework of a study agreement with Sofia University, meeting the specifics of the major and with 4 or more (ECTS) credits awarded, may be recognized and enlisted in the diploma as electives instead of those included in the present curriculum.*

Internships

№	code				Internship	Type – C, E, O	Semester	ECTS credits	Weeks	Hours	Type of grading* - e, ca, m
1	I	0	1	0	Research practicum	**C**	**3**	**10**	**15**	**300**	**ca**

Degree completion

Form of degree completion	ECTS credits	First session for thesis defence	Second session for thesis defence
Master thesis defence	15	February-March	July-September

The curriculum has been approved by the Faculty Council, Record of Proceedings № 12 from 25.02.2025

DEAN:..........................

Type of grading:
e-exam, ca-current assesment,
m-matriculation,
a-advances to the next semester

The Faculty Council has decided that min. 50% of the total education load is independent study of the students

Sofia University "St. Kliment Ohridski"

Curriculum Reference Statement

Area of Study "Computer Chemistry"

Master's Degree Programme "Computational chemistry - in English"

Form of study: full-time; Length of study: three semesters

In-class course load, ECTS credits and courses completed per semester

Type of courses	I semester			II semester			III semester			Total		
	Course Load - number of hours	ECTS credits	Number of grades	Course Load - number of hours	ECTS credits	Number of grades	Course Load - number of hours	ECTS credits	Number of grades	Course Load - number of hours	ECTS credits	Number of grades
Core courses	**360**	**30**	**5**	**390**	**26**	**5**	**60**	**5**	**1**	**810**	**61**	**11**
Min. of elective courses				**60**	**4**	**1**				**60**	**4**	**1**
internships							**150**	**10**	**1**	**150**	**10**	**1**
Total:	**360**	**30**	**5**	**450**	**30**	**6**	**210**	**15**	**2**	**1020**	**75**	**13**

Form of degree completion	ECTS credits	Number of hours for preparation	First thesis defence session	Second thesis defence session
Master thesis defence	15	450	February-March	July-September

Acquired Professional Qualification: Master of Computer Chemistry - Computational Chemistry

Record of Proceedings of the Faculty Council № 12 from 25.02.2025

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