



SOFIA UNIVERSITY "ST. KLIMENT OHRIDSKI"

FACULTY OF CHEMISTRY AND PHARMACY

## CURRICULUM

Signed by: .....

Approved by the Academic Council,  
Record of Proceedings № 1

11 12 4 10 КУ 2015г.

Professional Field: 4.2 Chemistry

Educational and Qualification Degree: Master of Science

Subject Area: Computer chemistry

Master programme: Computational chemistry

C	H	C	2	5	2	4	1	5
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Form of Study: full-time

Length of Study: 3 semesters

Professional Qualification: Master in Computer chemistry – Computational chemistry

C	2	5	2	4
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CHC252415

### Major "Computer Chemistry" / M. Sc. Program "Computational Chemistry"

for the academic year beginning in 2015

№	Course code	Course Title	Type – C, E, O	Semester	ECTS credits	Number of hours- total				Number of hours per week	Type of grading* - e, ca, m, a
						Total	Lectures	Seminars	Practical classes		
1	2	3	4	5	6	7	8	9	10	11	12

#### Core courses

1	C 0 1 8	Quantum chemistry for molecular systems	C	1	8	240	60	-	45	7	e
2	C 0 2 6	Molecular modelling with QSAR	C	1	6	180	45	-	30	5	e
3	C 0 3 6	Scientific programming	C	1	6	180	30	-	45	5	e
4	C 0 4 4	Molecular mechanics	C	1	4	120	30	-	15	3	e
5	C 0 5 6	Term project	C	1	6	180	15	-	45	4	ca
6	C 0 6 5	Quantum-chemical methods for periodic and nanostructures	C	2	5	150	45	-	15	4	e
7	C 0 7 4	Hybrid (QM/MM) methods	C	2	4	120	30	-	30	4	e
8	C 0 8 4	Computational methods in spectroscopy	C	2	4	120	30	-	30	4	e
9	C 0 9 5	Molecular dynamics and Monte Carlo simulations	C	2	5	150	30	-	30	4	e
10	C 1 0 9	Applied computational chemistry	C	2	9	270	30	-	105	9	ca
11	C 1 1 4	Analysis, reference and presentation of theoretical studies	C	3	4	120	30	-	30	4	ca

#### Elective courses – courses with minimum of 4 ECTS (total) must be elected

1	E 0 1 4	Modelling of chemical processes (neural networks in chemistry)	E	2	4	120	30	-	30	4	e
2	E 0 2 4	Molecular kinetics and thermodynamics by ab initio MO calculations	E	2	4	120	30	-	30	4	e

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

3	E	0	3	4	Introduction to programming in Linux shells and data processing	E	2	4	120	30	-	30	4	e
4	E	0	4	4	Object-oriented programming*	E	2	4	120	30	-	30	4	e
5	E	0	5	4	Ecometrics*	E	2	4	120	45	-	15	4	e
6	E	0	6	4	Symmetry of molecules and crystals	E	2	4	120	30	-	30	4	e
7	E	0	7	4	Biophysical chemistry*	E	2	4	120	30	-	30	4	e
8	E	0	8	4	Applied mass spectrometry*	E	2	4	120	30	-	30	4	e
9	E	0	9	4	Structure and properties of materials*	E	2	4	120	30	-	30	4	e
10	E	1	0	4	X-ray analysis *	E	2	4	120	30	-	30	4	e
11	E	1	1	4	Optical and electron microscopy*	E	2	4	120	30	-	30	4	e
12	E	1	2	4	Methods for nanomaterials characterization*	E	2	4	120	30	-	15	3	e
13	E	1	3	4	Modeling of nanostructures*	E	2	4	120	30	-	15	3	e
14	E	1	4	4	Biological macromolecuels*	E	2	4	120	30	-	15	3	e
15	E	1	5	4	Bioelectronics*	E	2	4	120	30	-	30	4	e
16	E	1	6	4	Chemistry and physics of luminophores*	E	2	4	120	15	-	15	2	e
17	E	1	7	4	Spectroscopic methods for characterization*	E	2	4	120	30	-	30	4	e
18	E	1	8	4	Applied organic photochemistry*	E	2	4	120	45	-	15	4	e
19	E	1	9	4	Coordination compounds and their application in modern technologies*	E	2	4	120	30	-	30	4	e
20	E	2	0	4	Theory and computer modeling of polymers*	E	2	4	120	30	-	30	4	e
21	E	2	1	4	Photochemistry*	E	2	4	120	30	-	30	4	e
22	E	2	2	4	X-ray fluorecence analysis*	E	2	4	120	15	-	30	3	e
23	E	2	3	4	Modern techniques in NMR spectroscopy*	E	2	4	120	30	-	30	4	e
24	E	2	4	4	Modern methods of molecular spectroscopy*	E	1	4	120	30	-	30	4	e
25	E	2	5	4	Multivariant statistics in chemical analysis*	E	1	4	120	30	-	30	4	e

\* Course from another M.Sc. Program

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

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Study Internships									
No	code	Internship	Type - C, E, O	Semester	ECTS credits	Weeks	Hours	Type of grading* - e, ca, m	
1	1012	Pre-thesis training	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	15	February-March	June-July

The curriculum has been approved by the Faculty Council, Record of Proceedings № 5/18.11.2014

DEAN:.....

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

Sofia University "St. Kliment Ohridski"

**Curriculum Reference Statement**

M. Sc. Program "Computational chemistry"

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
Compulsory courses	360	30	5	375	27	5	60	4	1	795	61	11
Min. of elective courses				60	4	1				60	4	1
Study internships							150	10	1	150	10	1
<b>Total:</b>	<b>360</b>	<b>30</b>	<b>5</b>	<b>435</b>	<b>31</b>	<b>6</b>	<b>210</b>	<b>14</b>	<b>2</b>	<b>1005</b>	<b>75</b>	<b>13</b>

Degree completion	ECTS credits	Number of hours for preparation	First state exam/ thesis defence session	Second state exam/ thesis defence session
Master thesis	15	300	February-March	June-July

**Professional Qualification:** Master of Computer Chemistry - Computational Chemistry

**Record of Proceedings of the Faculty Council № 5/18.11.2014**

**Dean:**