

Graduate program: Chemistry, MSc program “Computational chemistry”**Degree awarded: Master of Science (MSc)*****Admission requirements***

The applicants should be holders of BSc or MSc degree in chemistry, physics, biology or biotechnology awarded from the University of Sofia or other universities and all majors from the University for chemical technology and metallurgy or from the Technical universities. An admission test in chemistry should be taken for state-subsidized education (available for Bulgarian students only). Rating includes the marks from the admission test, from the last diploma defense and from the average academic grades. Students in self-subsidized form of education are admitted on the basis of their average academic grades only. Details about the admission of foreign students could be found at the website: <http://www.uni-sofia.bg/students/admission/foreign.html>

Goals***Educational***

Advanced theoretical background in: quantum chemical methods for simulation of atoms, molecules and crystals; molecular structure-property relationship; molecular mechanics and molecular dynamics; design of materials with predefined properties; prediction and analysis of molecular spectra; mechanism of chemical reactions at molecular level.

These educational goals are achieved by appropriate lecture and practical courses focused on the basic theoretical methods and on the composition-structure-properties relationships of compounds.

Professional

Training of individuals with detailed in-depth knowledge in the area of computational chemistry as well as with specific practical skills for analysis of numerical results from commercial scientific software packages, prediction of materials properties, and literacy in scientific programming with various programming languages.

Career opportunities

The MSc in Computational chemistry awardees can continue their education as PhD students in the same or related scientific field or join various research teams in theoretical chemistry worldwide. They can also make industry-oriented career in: organic synthesis, pharmaceuticals, biotechnology, micro- and optoelectronics, lasers, environmental protection, nanotechnology, catalysis, materials science and technology.

Curriculum with ECTS credits (90 for the entire MSc program)

First year					
First semester			Second semester		
Course code and course title	ECTS credits	Type of course	Course code and course title	ECTS credits	Type of course
		C or E	C = Compulsory E = Elective		
Quantum chemistry for molecular systems	8	C	Quantum-chemical methods for periodic and nanostructures	5	C

Molecular modeling and QSAR	6	C	Modeling of chemical processes (neural networks in chemistry)	4	C
Introduction to FORTRAN	6	C	Computational methods in spectroscopy	5	C
Molecular mechanics	4		Molecular dynamics and Monte Carlo simulations	5	C
Term project	5	C	Research practicum	10	C
Symmetry of molecules and crystals	4	E	Ab initio MO computations	4	E
Chemometry ²	4	E	Hybrid QM/MM methods	4	E
			Object-oriented programming ³	4	E

Second year					
Third semester			Fourth semester		
Course code and course title	ECTS credits	Type of course	Course code and course title	ECTS credits	Type of course
Prethesis training	8	C			
M. Sc. Thesis	20	C			
* One elective course is mandatory to fit the total of 90 ECTS credits required for the entire MSc program.					
<i>General remarks:</i>					
1. Electives can be taken in any semester. Courses from other MSc programs are allowed. The number of electives is not limited.					
2. Course from another MSc program.					
3. Elective at the Faculty of Mathematics and Informatics.					

Examination and assessment regulations

Written tests for all disciplines. Additional requirements for final grade formation are formulated in each detailed course description.

Final examination

Public MSc diploma thesis defense

Technical equipment and facilities

Four computer classes (one of them equipped with multimedia setup) and one computer cluster are on hand at the Faculty of Chemistry. Two computer clusters at the Institutes of Catalysis of Physical Chemistry of BAS are accessible too. These facilities are provided with adequate software for the tuition in the MSc program. Hardware available: 30 Pentium PCs, 4 workstations, 3 computer clusters. Software offered: GAUSSIAN, MOPAC, GAMESS, CHEMOFFICE, CHEM-X, HYPERCHEM, CRYSTAL, and other commercial and original codes. The computer lab facilities give each student access to information sources. The research activity of the lecturers provides right to use databases and literature sources outside Bulgaria.

Research areas of the lecturers

The teachers are qualified in scientific areas related to the subjects taught. Their research interests are predominantly in the field of: structure, energy spectrum, electric, optical and magnetic properties of molecules and molecular assemblies with reference to design of new

materials; quantum dynamics on solid surfaces at nanoscopic level; crystal growth and heterogeneous catalysis; modeling of biocompatibility and chemistry of biodegradability (QSAR); computer simulations of living polymers; conformational search of bioorganic molecules; molecular machines.

Some of the lecturers are leaders or experts in various research project teams or participate in national, European or global expert panels, international associations and in the editorial boards of international journals.

Specifics of the credit system implementation

Most of the courses require individual term project preparation credits for which are allocated in the respective course descriptions. The practical courses XXX are organized as lab exercises (mandatory) and carry credits as described in the curriculum. Each extracurricular elective adds 4 extra credits. Participation in scientific forums accumulates 4 (oral) or 2 (poster) extra credits.

ECTS departmental coordinator

Assoc. Prof. Dr. Nikolay Denkov, Vice Dean of the Faculty of Chemistry
