

COURSES IN FOREIGN LANGUAGES for ERASMUS INCOMING STUDENTS

Sofia University 2020/2021 academic year

Faculty of Chemistry and Pharmacy

Faculty coordinator: Prof. Todor Dudev, t.dudev@chem.uni-sofia.bg

Programme: Bachelor program Chemistry

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX010113 3257	Polymers	English	BSc	Summer	7	45		45	Assoc. Prof. L. Hristov	christov@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): An introductory course in polymer science as an important part of material science. With an emphasis on polymer chemistry and synthesis, the course explains some basic physical properties and the methods for characterization and processing of polymers.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX010113 IIA10	Biocoordination chemistry	English	BSc	Summer	5	30		30	Assoc. Prof. A. Ahmedova	ahaa@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The modern bioinorganic (biocoordination) chemistry deals with the biological processes involving metalloenzymes and metalloproteins, focusing on the main structural and functional characteristics related to the presence of metal ion(s) in their active site. This involves deeper understanding of the properties of metal ions to form coordination compounds and the corresponding characteristics of their structure and reactivity that are directly connected with the biological activity. Another crucial subject of

the bioinorganic chemistry is the application of metal complexes in medicine for diagnostics and therapy of wide range of diseases. The unique properties of the metal complexes and the knowledge about the structure-reactivity-biological activity relationship hold out the opportunity for intelligent design of metallopharmaceuticals with target properties and activity. That is why the subjects in the present teaching course will evolve from the fundamental coordination chemistry knowledge to the direct pharmaceutical applications of metal complexes as therapeutic or diagnostic agents including quickly developing field of radiopharmaceuticals. The students will have the opportunity to synthesize by themselves the first metal-based chemotherapeutics, the cisplatin, during the practical work of this course.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦЯ030113 ИH09	Methods for dating of archaeological and geological materials	English	BSc	Winter/ Summer	5	30		30	Assoc. Prof. Petya Kovacheva	nhpk@wmail.chem.uni-sofia.bg

Short description of the course: The course acquaints the students with the methods for absolute and relative dating of different archeological finds (bones, wood, charcoal, ceramics, textile, paper) and geological materials (rocks, minerals, stalactites, stalagmites). Among the methods discussed are: potassium-argon method, radiocarbon, radiocalcium, uranium series, thermoluminescence, fission track method, racemization of aminoacids, isochron dating, dendrochronology, archaeomagnetism, obsidian hydration dating etc. The principle of each method, requirements for sampling, sample preparation and measurement techniques are described. General possibilities and limits of the dating methods are discussed. Examples of dated popular archaeological and geological objects are given to illustrate the applicability of the methods.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX010113 ИФ07	Molecular Design	English	BSc	Summer	5	30		30	Prof. A. Tadjer	tadjer@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): Molecular systems with predefined physical and chemical characteristics and/or biological activity are intensively sought both experimentally and theoretically. The course introduces the main classes of materials of interest for modern technologies, cosmetics, and pharmacy. The rules and schemes of QSPR are presented with accent on the design of compounds with potential for utilization into technology, pharmacy, and ecology. During the computational practicum each student is assigned an individual project

aimed at modelling of a prospective compound from one of the above-mentioned groups. Specialized software and a wide range of computational methods are applied. The results are discussed and summarized into a term project, which is presented and defended in front of a professional audience at the end of the semester.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX010113 ИФ16	Molecular Modelling of Functional Materials	English	BSc	Summer	5	30		30	Assoc. Prof. G. Madjarova	gmadjarova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course focuses on the application of quantum chemical methods for description of the relationships between the structure and properties of modern functional materials at the molecular level. The lectures introduce students to the mechanisms responsible for the specific characteristics of functional materials and outline the techniques for modelling them theoretically. Using Density Functional Theory, a set of quantities required for assessment of various physical and chemical molecular properties are calculated. The results obtained during the computational practicum for an individually assigned molecule are summarized into a written term project, which is submitted at the end of the semester. The knowledge obtained from the course enables students to perform directed molecular modelling of new more efficient, cheaper, more environmentally friendly, and durable materials.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX010113 ИФ09	Quantum Chemistry	English	BSc	Winter/ Summer	5	30		30	Prof. A. Tadjer	tadjer@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course acquaints students with the contemporary methods of quantum chemistry and their capacity for application to estimate molecular properties. The methods allowing theoretical determination of molecular characteristics such as geometry, electron density, and energy spectrum are presented. The theoretical foundation and the basic formalism of the methods are summarized and the areas of applicability are discussed. Appropriate illustrative examples are included. Both the lectures and the computational exercises are practically oriented. Each student is assigned an individual term project, which is summarized, submitted in writing and presented orally at the end of the semester. After completing the course students are able to carry out independently a

basic computational study of a particular chemical or theoretical problem and to analyze adequately the obtained numerical data using the appropriate specialized software.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX010113 313	Structure of Matter	English	BSc	Winter	6	45		30	Prof. A. Tadjer Assoc. Prof. G. Madjarova Prof. A. Ivanova	tadjer@chem.uni-sofia.bg gmadjarova@chem.uni-sofia.bg aivanova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course is offered in several versions containing different numbers of academic hours and of ECTS assigned. It encompasses the part of chemistry, which addresses the description of chemical characteristics at the microscopic level. The lectures introduce basic concepts and terms of quantum mechanics and demonstrate their application to chemical objects. The knowledge, which allows prediction of chemical characteristics and theoretical interpretation of the behaviour of real discrete systems is presented. The topics include: energy spectra of atoms and molecules; nature of chemical bonding; molecular structure and electron density; intermolecular forces, hydrogen bonds, modulating effects of the environment, etc. The symmetry apparatus is taught and practiced. During the computational practicum students acquire hands-on experience with basic computational software by using it to calculate molecular properties of an individually assigned molecule. All results are summarized at the end of the semester and presented and discussed during a written test. After completing the course students are familiar with the fundamental concepts of the structure of matter, are able to apply them for interpreting chemical properties at the molecular level, and understand and discuss the outcome of simple molecular simulations.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		

XΦX010113 И01Φ	Application of Statistics in Molecular Modelling	English	BSc	Summer	5	45		15	Prof. A. Ivanova	aivanova@chem.uni-sofia.bg
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Short description of the course (done in the language of instruction): The course enables students to apply basic approaches for statistical analysis to datasets obtained from molecular modelling. The lectures introduce basic concepts of molecular modelling with focus on collection and processing of numerical data yielded by multiple-step molecular simulations. The main goal is presentation of the techniques for statistical analysis of such data arrays. The sources of and methods for estimation of statistical errors are reviewed. The exercises are oriented towards practical mastering of these techniques. Software products for statistical analysis are learned and competences for evaluation of molecular properties by statistical assessment are developed. After completing the course students are able to apply methods for statistical analysis on temporal and other datasets, to extract characteristics of chemical objects and to interpret the physical meaning of the obtained numerical estimates.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX010113 И009	Optical properties of functional organic compounds	English	BSc	Summer	5	30	30		Assoc. Prof. St. Stoyanov	ohss@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course gives the students an opportunity to expand their knowledge on the fundamental rules which connect the optical properties of organic compounds and their structure. The main approaches towards designed synthesis of organic compounds with desired photophysical properties are discussed along with theoretical and practical training in some of the most powerful "state-of-the-art" spectroscopic techniques and photochemical methods. Special attention will be paid on the reflectance spectroscopy and perception of color, and also on the real-life applications of specific structures for optical sensing, light harvesting, etc. In summary, the course aims at building bridges between the most common spectroscopic methods, the organic compounds' structure, the fine tuning of their optical properties, and their hi-tech applications.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX010113 И050	Organic Photochemistry	English	BSc	Winter	5	45	15		Assoc. Prof. St. Stoyanov	ohss@chem.uni-sofia.bg

Short description of the course (done in the language of instruction)										
The course aims at getting the students acquainted with the structural specifics and reactivity of organic molecules in their electronically excited state, as well as some applications of the light-matter interactions. The main accent is the comparison between thermal and light induced activation in the case of different classes of organic compounds, e.g. carbonyls, alkenes, dienes, arenes, etc. The pros and cons of using UV/Vis light as initiator of reactions without analog in the “classic” organic synthesis are also discussed.										
Requirements for enrollment: NO										
Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX010113 I06A	Chemometrics	English	BSc	Summer	5	45	30		Prof. S. Tsakovski	STsakovski@chem.uni-sofia.bg
Short description of the course (done in the language of instruction): The course focuses on the application of traditional methods of classical and multivariate statistics as a tool for assessment, classification, interpretation and modelling of data sets obtained from chemical, environmental and clinical studies. The practical exercises are based on real-life data sets and include assessment of analytical procedures, design of experiments, exploratory and modelling analysis. The results are discussed and summarized into a term project, which is defended at the end of the course.										
Requirements for enrollment: NO										
Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX010113 3247	Modern Instrumental Methods for Analysis - Molecular Spectroscopy and Magnetic Methods	English	BSc	Summer	7	60		45	Assoc. Prof. Gencheva	ahgg@chem.uni-sofia.bg
Short description of the course (done in the language of instruction): The aim of this course is to give a theoretical and practical introduction into selected instrumental analytical methods (UV-Vis and molecular fluorescence spectroscopy, Fourier Transform Infrared (FT-IR) and Raman spectroscopy, circular dichroism, magnetic resonance spectroscopy: NMR and ESR) as well as to present the opportunities for their contemporary application in structural and quantitative characterization of chemicals, bio-molecules and bio-conjugates, polymers, materials, surfaces, etc. The										

goal of the course is to equip students with practical skills for interpretation of spectra and data and thus to enable them in using of the presented methods in their research work.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX010113 ИA08	Vibrational Spectroscopy – methods and application (elective)	English	BSc	Summer	4	30		30	Assoc. Prof. Gencheva	ahgg@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): In-depth course on the principal of vibrational spectroscopy: Fourier Transform Infrared (FT-IR) spectroscopy, IR-Microscopy, FT-Raman spectroscopy and their use in solving problems of structural, functional and quantitative analysis of organic, organometallic and inorganic compounds.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX010113 И02Φ	Quantum Chemistry and Molecular Mechanics	English	BSc	Winter/ Summer	5	45		15	Assoc. Prof. G. Madjarova	gmadjarova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course acquaints students with the modern methods of quantum chemistry and molecular mechanics that allow theoretical determination of molecular characteristics: conformational search, geometry, electronic densities, energy spectrum. The program includes a general introduction of the main classes of modern quantum-chemical methods and discusses their application limits. The potential functions and parameters of the molecular mechanical force field are also discussed. Specific illustrative examples are provided. Lectures and exercises are practically oriented. Each student receives an individual course project.

Requirements for enrollment: NO

Programme: Bachelor program ECO Chemistry

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦE020113 IA10	Biocoordination chemistry (elective)	English	BSc	Summer	5	30		30	Assoc. Prof. A. Ahmedova	ahaa@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The modern bioinorganic (biocoordination) chemistry deals with the biological processes involving metalloenzymes and metalloproteins, focusing on the main structural and functional characteristics related to the presence of metal ion(s) in their active site. This involves deeper understanding of the properties of metal ions to form coordination compounds and the corresponding characteristics of their structure and reactivity that are directly connected with the biological activity. Another crucial subject of the bioinorganic chemistry is the application of metal complexes in medicine for diagnostics and therapy of wide range of diseases. The unique properties of the metal complexes and the knowledge about the structure-reactivity-biological activity relationship hold out the opportunity for intelligent design of metallopharmaceuticals with target properties and activity. That is why the subjects in the present teaching course will evolve from the fundamental coordination chemistry knowledge to the direct pharmaceutical applications of metal complexes as therapeutic or diagnostic agents including quickly developing field of radiopharmaceuticals. The students will have the opportunity to synthesize by themselves the first metal-based chemotherapeutics, the cisplatin, during the practical work of this course.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦЯ030113 IH09	Methods for dating of archaeological and geological materials	English	BSc	Winter/ Summer	5	30		30	Assoc. Prof. Petya Kovacheva	nhpk@wmail.chem.uni-sofia.bg

Short description of the course: The course acquaints the students with the methods for absolute and relative dating of different archeological finds (bones, wood, charcoal, ceramics, textile, paper) and geological materials (rocks, minerals, stalactites, stalagmites). Among the methods discussed are: potassium-argon method, radiocarbon, radiocalcium, uranium series, thermoluminescence, fission track method, racemization of aminoacids, isochron dating, dendrochronology, archaeomagnetism, obsidian hydration dating etc. The principle of each method, requirements for sampling, sample preparation and measurement techniques are described. General possibilities and limits of the dating methods are discussed. Examples of dated popular archaeological and geological objects are given to illustrate the applicability of the methods.

Requirements for enrollment: NO										
Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦE020113 ИФ07	Molecular Design	English	BSc	Summer	5	30		30	Prof. A. Tadjer	tadjer@chem.uni-sofia.bg
<p>Short description of the course (done in the language of instruction): Molecular systems with predefined physical and chemical characteristics and/or biological activity are intensively sought both experimentally and theoretically. The course introduces the main classes of materials of interest for modern technologies, cosmetics, and pharmacy. The rules and schemes of QSPR are presented with accent on the design of compounds with potential for utilization into technology, pharmacy, and ecology. During the computational practicum each student is assigned an individual project aimed at modelling of a prospective compound from one of the above-mentioned groups. Specialized software and a wide range of computational methods are applied. The results are discussed and summarized into a term project, which is presented and defended in front of a professional audience at the end of the semester.</p>										
Requirements for enrollment: NO										
Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦE020113 ИФ10	Molecular Modelling of Functional Materials	English	BSc	Summer	5	30		30	Assoc. Prof. G. Madjarova	gmadjarova@chem.uni-sofia.bg
<p>Short description of the course (done in the language of instruction): The course focuses on the application of quantum chemical methods for description of the relationships between the structure and properties of modern functional materials at the molecular level. The lectures introduce students to the mechanisms responsible for the specific characteristics of functional materials and outline the techniques for modelling them theoretically. Using Density Functional Theory, a set of quantities required for assessment of various physical and chemical molecular properties are calculated. The results obtained during the computational practicum for an individually assigned molecule are summarized into a written term project, which is submitted at the end of the semester. The knowledge obtained from the course enables students to perform directed molecular modelling of new more efficient, cheaper, more environmentally friendly, and durable materials.</p>										
Requirements for enrollment: NO										

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦE020113 ИΦ03	Quantum Chemistry	English	BSc	Winter/ Summer	5	30		30	Prof. A. Tadjer	tadjer@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course acquaints students with the contemporary methods of quantum chemistry and their capacity for application to estimate molecular properties. The methods allowing theoretical determination of molecular characteristics such as geometry, electron density, and energy spectrum are presented. The theoretical foundation and the basic formalism of the methods are summarized and the areas of applicability are discussed. Appropriate illustrative examples are included. Both the lectures and the computational exercises are practically oriented. Each student is assigned an individual term project, which is summarized, submitted in writing and presented orally at the end of the semester. After completing the course students are able to carry out independently a basic computational study of a particular chemical or theoretical problem and to analyse adequately the obtained numerical data using the appropriate specialized software.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦE020113 3185	Structure of Matter	English	BSc	Winter	5	30		30	Prof. A. Tadjer Assoc. Prof. G. Madjarova Prof. A. Ivanova	tadjer@chem.uni-sofia.bg gmadjarova@chem.uni-sofia.bg aivanova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course is offered in several versions containing different numbers of academic hours and of ECTS assigned. It encompasses the part of chemistry, which addresses the description of chemical characteristics at the microscopic level. The lectures introduce basic concepts and terms of quantum mechanics and demonstrate their application to chemical objects. The knowledge, which allows prediction of chemical characteristics and theoretical interpretation of the behaviour of real discrete systems is presented.

The topics include: energy spectra of atoms and molecules; nature of chemical bonding; molecular structure and electron density; intermolecular forces, hydrogen bonds, modulating effects of the environment, etc. The symmetry apparatus is taught and practiced. During the computational practicum students acquire hands-on experience with basic computational software by using it to calculate molecular properties of an individually assigned molecule. All results are summarized at the end of the semester and presented and discussed during a written test. After completing the course students are familiar with the fundamental concepts of the structure of matter, are able to apply them for interpreting chemical properties at the molecular level, and understand and discuss the outcome of simple molecular simulations.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦE020113 IO09	Optical properties of functional organic compounds	English	BSc	Summer	5.5	30	30		Assoc. Prof. St. Stoyanov	ohss@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course gives the students an opportunity to expand their knowledge on the fundamental rules which connect the optical properties of organic compounds and their structure. The main approaches towards designed synthesis of organic compounds with desired photophysical properties are discussed along with theoretical and practical training in some of the most powerful "state-of-the-art" spectroscopic techniques and photochemical methods. Special attention will be paid on the reflectance spectroscopy and perception of color, and also on the real-life applications of specific structures for optical sensing, light harvesting, etc. In summary, the course aims at building bridges between the most common spectroscopic methods, the organic compounds' structure, the fine tuning of their optical properties, and their hi-tech applications.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦE020113 3257	Modern Instrumental Methods for Analysis - Molecular Spectroscopy and Magnetic Methods	English	BSc	Summer	7	45		45	Assoc. Prof. Gencheva	ahgg@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The aim of this course is to give a theoretical and practical introduction into selected instrumental analytical methods (UV-Vis and molecular fluorescence spectroscopy, Fourier Transform Infrared (FT-IR) and Raman spectroscopy, circular dichroism, magnetic resonance spectroscopy: NMR and ESR) as well as to present the opportunities for their contemporary application in structural and quantitative characterization of chemicals, bio-molecules and bio-conjugates, polymers, materials, surfaces, etc. The goal of the course is to equip students with practical skills for interpretation of spectra and data and thus to enable them in using of the presented methods in their research work.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦE020113 IIA08	Vibrational Spectroscopy – methods and application	English	BA	Summer	4	30		30	Assoc. Prof. Gencheva	ahgg@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): In-depth course on the principal of vibrational spectroscopy: Fourier Transform Infrared (FT-IR) spectroscopy, IR-Microscopy, FT-Raman spectroscopy and their use in solving problems of structural, functional and quantitative analysis of organic, organometallic and inorganic compounds.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX010113 II02Φ	Quantum Chemistry and Molecular Mechanics	English	BSc	Winter/ Summer	5	45		15	Assoc. Prof. G. Madjarova	gmadjarova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course acquaints students with the modern methods of quantum chemistry and molecular mechanics that allow theoretical determination of molecular characteristics: conformational search, geometry, electronic densities, energy spectrum. The program includes a general introduction of the main classes of modern quantum-chemical methods and discusses their application limits. The potential functions and parameters of the molecular mechanical force field are also discussed. Specific illustrative examples are provided. Lectures and exercises are practically oriented. Each student receives an individual course project.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX010113 И01Φ	Application of Statistics in Molecular Modelling	English	BSc	Summer	5	45		15	Prof. A. Ivanova	aivanova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course enables students to apply basic approaches for statistical analysis to datasets obtained from molecular modelling. The lectures introduce basic concepts of molecular modelling with focus on collection and processing of numerical data yielded by multiple-step molecular simulations. The main goal is presentation of the techniques for statistical analysis of such data arrays. The sources of and methods for estimation of statistical errors are reviewed. The exercises are oriented towards practical mastering of these techniques. Software products for statistical analysis are learned and competences for evaluation of molecular properties by statistical assessment are developed. After completing the course students are able to apply methods for statistical analysis on temporal and other datasets, to extract characteristics of chemical objects and to interpret the physical meaning of the obtained numerical estimates.

Requirements for enrollment: NO

Programme: Bachelor program Computer Chemistry

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦK040113 ИA10	Biocoordination chemistry (elective)	English	B. Sc./ MSci	Summer/ Winter	5	30		30	Assoc. Prof. A. Ahmedova	ahaa@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The modern bioinorganic (biocoordination) chemistry deals with the biological processes involving metalloenzymes and metalloproteins, focusing on the main structural and functional characteristics related to the presence of metal ion(s) in their active site. This involves deeper understanding of the properties of metal ions to form coordination compounds and the corresponding characteristics of their structure and reactivity that are directly connected with the biological activity. Another crucial subject of the bioinorganic chemistry is the application of metal complexes in medicine for diagnostics and therapy of wide range of diseases. The unique properties of the metal complexes and the knowledge about the structure-reactivity-biological activity relationship hold out the opportunity for intelligent design of metallopharmaceuticals with target properties and activity. That is why the subjects in the present teaching course will evolve

from the fundamental coordination chemistry knowledge to the direct pharmaceutical applications of metal complexes as therapeutic or diagnostic agents including quickly developing field of radiopharmaceuticals. The students will have the opportunity to synthesize by themselves the first metal-based chemotherapeutics, the cisplatin, during the practical work of this course.\

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦЯ030113 ИH09	Methods for dating of archaeological and geological materials	English	BSc	Winter/ Summer	5	30		30	Assoc. Prof. Petya Kovacheva	nhpk@wmail. chem.uni- sofia.bg

Short description of the course: The course acquaints the students with the methods for absolute and relative dating of different archeological finds (bones, wood, charcoal, ceramics, textile, paper) and geological materials (rocks, minerals, stalactites, stalagmites). Among the methods discussed are: potassium-argon method, radiocarbon, radiocalcium, uranium series, thermoluminescence, fission track method, racemization of aminoacids, isochron dating, dendrochronology, archaeomagnetism, obsidian hydration dating etc. The principle of each method, requirements for sampling, sample preparation and measurement techniques are described. General possibilities and limits of the dating methods are discussed. Examples of dated popular archaeological and geological objects are given to illustrate the applicability of the methods.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦK040113 ИΦ07	Molecular Design	English	BSc	Summer	5	30		30	Prof. A. Tadger	tadger@chem. uni-sofia.bg

Short description of the course (done in the language of instruction): Molecular systems with predefined physical and chemical characteristics and/or biological activity are intensively sought both experimentally and theoretically. The course introduces the main classes of materials of interest for modern technologies, cosmetics, and pharmacy. The rules and schemes of QSPR are presented with accent on the design of compounds with potential for utilization into technology, pharmacy, and ecology. During the computational practicum each student is assigned an individual project aimed at modelling of a prospective compound from one of the above-mentioned groups. Specialized software and a wide range of computational methods are applied. The results are discussed and summarized into a term project, which is presented and defended in front of a professional audience at the end of the semester.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦK040113 ИФ16	Molecular Modelling of Functional Materials	English	BSc	Summer	5	30		30	Assoc. Prof. G. Madjarova	gmadjarova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course focuses on the application of quantum chemical methods for description of the relationships between the structure and properties of modern functional materials at the molecular level. The lectures introduce students to the mechanisms responsible for the specific characteristics of functional materials and outline the techniques for modelling them theoretically. Using Density Functional Theory, a set of quantities required for assessment of various physical and chemical molecular properties are calculated. The results obtained during the computational practicum for an individually assigned molecule are summarized into a written term project, which is submitted at the end of the semester. The knowledge obtained from the course enables students to perform directed molecular modelling of new more efficient, cheaper, more environmentally friendly, and durable materials.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦK040113 ИФ09	Quantum Chemistry	English	BSc	Winter/ Summer	5	30		30	Prof. A. Tadger	tadger@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course acquaints students with the contemporary methods of quantum chemistry and their capacity for application to estimate molecular properties. The methods allowing theoretical determination of molecular characteristics such as geometry, electron density, and energy spectrum are presented. The theoretical foundation and the basic formalism of the methods are summarized and the areas of applicability are discussed. Appropriate illustrative examples are included. Both the lectures and the computational exercises are practically oriented. Each student is assigned an individual term project, which is summarized, submitted in writing and presented orally at the end of the semester. After completing the course students are able to carry out independently a basic computational study of a particular chemical or theoretical problem and to analyze adequately the obtained numerical data using the appropriate specialized software.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s`s E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦK040113 3157	Theoretical Chemistry	English	BSc	Winter	7	45		45	Prof. A. Tadjer Assoc. Prof. G. Madjarova Prof. A. Ivanova	tadjer@chem.uni-sofia.bg gmadjarova@chem.uni-sofia.bg aivanova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course encompasses the part of Physical chemistry related to the properties of microscopic systems. It presents a short overview of basic concepts and ideas of quantum mechanics and demonstrates their application to chemical objects. The main objective of the course is to provide fundamental and applied knowledge for prediction of molecular characteristics and interpretation of the behaviour of real systems. Concepts such as nature of chemical bonding, geometry of molecules, electron density distribution, and energy spectra are clarified. A separate chapter is devoted to the description of weak intermolecular interactions, hydrogen bonds, environment effects. The role of symmetry for solving chemical problems is outlined. The computational exercises comprise practice with software products to calculate molecular properties. Each student is assigned an individual molecule, the results for which are summarized and submitted as a term project at the end of the semester.

Upon completion of the course students consolidate and broaden their knowledge on atomic structure, nature and specifics of chemical bonds, structure-property relationships, influence of the environment and capabilities for molecular modelling of processes and materials. The basic logics of software products for molecular simulations is familiar.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s`s E-mail
						Lectures	Exercises/ Seminars	Practical work		

XΦK040113 3278	Bioorganic Chemistry	English	BSc	Summer	8	60	45		Prof. Todor Dudev	t.dudev@che m.uni-sofia.bg
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Short description of the course (done in the language of instruction): The course is intended to provide a general knowledge on the structure and properties of the basic bioorganic molecules such as proteins, nucleic acids, carbohydrates, lipids, hormones/neurotransmitters and vitamins. Special attention will be given to the processes regulating the vital processes in the cell such as respiration, food assimilation, signal transduction, protein synthesis, muscle contraction, blood coagulation and enzyme activation.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s` E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦK040113 3226	Instrumental Methods for Analysis	English	BSc	summer	6	45	30		Prof. Todor Dudev	t.dudev@che m.uni-sofia.bg

Short description of the course (done in the language of instruction): The students will acquire basic knowledge and skills in applying instrumental methods in solving various problems in chemistry and pharmaceutical chemistry. Methods such as UV/VIS, Fluorescence, Infrared, Raman, NMR spectroscopy and Mass spectrometry are included. As a result of the successful completion of the course students will be able to perform both quantitative and qualitative analyses of the samples of interest as well as choose the most appropriate approach to solve the analytical problem.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s` E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦK040113 3266	Quantitative structure- activity relationship (QSAR)	English	BSc	Summer	6	30	45		Assist. Prof. Diana Cheshmedzhi eva	dvalentinova @chem.uni- sofia.bg

Short description of the course (done in the language of instruction): The Quantitative Structure-activity relationship (QSAR) modeling is one of the major computational tools employed in medicinal chemistry and rational drug design. In the course students are introduced to some Molecular modeling methods that are relevant to drug design and 2D – and 3D – QSAR approaches. The students will learn how to build a QSAR model, how to choose between different models and how to interpret the data.

Requirements for enrollment: NO										
Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦK040113 IO09	Optical properties of functional organic compounds	English	BSc	Summer	5	30	30		Assoc. Prof. St. Stoyanov	ohss@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course gives the students an opportunity to expand their knowledge on the fundamental rules which connect the optical properties of organic compounds and their structure. The main approaches towards designed synthesis of organic compounds with desired photophysical properties are discussed along with theoretical and practical training in some of the most powerful "state-of-the-art" spectroscopic techniques and photochemical methods. Special attention will be paid on the reflectance spectroscopy and perception of color, and also on the real-life applications of specific structures for optical sensing, light harvesting, etc. In summary, the course aims at building bridges between the most common spectroscopic methods, the organic compounds' structure, the fine tuning of their optical properties, and their hi-tech applications.

Requirements for enrollment: NO										
Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦK040113 3256	Chemometrics	English	BSc	Full year	6	45	30		Prof. S. Tsakovski	STsakovski@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course focuses on the application of traditional methods of classical and multivariate statistics as a tool for assessment, classification, interpretation and modelling of data sets obtained from chemical, environmental and clinical studies. The practical exercises are based on real-life data sets and include assessment of analytical procedures, design of experiments, exploratory and modelling analysis. The results are discussed and summarized into a term project, which is defended at the end of the course.

Requirements for enrollment: NO										
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Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦK040113 IIA08	Vibrational Spectroscopy – methods and application	English	MSc	Summer	5	30		30	Assoc. Prof. Gencheva	ahgg@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): In-depth course on the principal of vibrational spectroscopy: Fourier Transform Infrared (FT-IR) spectroscopy, IR-Microscopy, FT-Raman spectroscopy and their use in solving problems of structural, functional and quantitative analysis of organic, organometallic and inorganic compounds.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX010113 II02Φ	Quantum Chemistry and Molecular Mechanics	English	BSc	Winter/ Summer	5	45		15	Assoc. Prof. G. Madjarova	gmadjarova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course acquaints students with the modern methods of quantum chemistry and molecular mechanics that allow theoretical determination of molecular characteristics: conformational search, geometry, electronic densities, energy spectrum. The program includes a general introduction of the main classes of modern quantum-chemical methods and discusses their application limits. The potential functions and parameters of the molecular mechanical force field are also discussed. Specific illustrative examples are provided. Lectures and exercises are practically oriented. Each student receives an individual course project.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		

XΦX010113 И01Φ	Application of Statistics in Molecular Modelling	English	BSc	Summer	5	45		15	Prof. A. Ivanova	aivanova@chem.uni-sofia.bg
<p>Short description of the course (done in the language of instruction): The course enables students to apply basic approaches for statistical analysis to datasets obtained from molecular modelling. The lectures introduce basic concepts of molecular modelling with focus on collection and processing of numerical data yielded by multiple-step molecular simulations. The main goal is presentation of the techniques for statistical analysis of such data arrays. The sources of and methods for estimation of statistical errors are reviewed. The exercises are oriented towards practical mastering of these techniques. Software products for statistical analysis are learned and competences for evaluation of molecular properties by statistical assessment are developed. After completing the course students are able to apply methods for statistical analysis on temporal and other datasets, to extract characteristics of chemical objects and to interpret the physical meaning of the obtained numerical estimates.</p>										
<p>Requirements for enrollment: NO</p>										

Programme: Bachelor program Chemical Engineering and Contemporary Materials

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX050113 ИA10	Biocoordination chemistry	English	BSc	Summer/ Winter	4	30		30	Assos. Prof. A. Ahmedova	ahaa@chem.uni-sofia.bg
<p>Short description of the course (done in the language of instruction): The modern bioinorganic (biocoordination) chemistry deals with the biological processes involving metalloenzymes and metalloproteins, focusing on the main structural and functional characteristics related to the presence of metal ion(s) in their active site. This involves deeper understanding of the properties of metal ions to form coordination compounds and the corresponding characteristics of their structure and reactivity that are directly connected with the biological activity. Another crucial subject of the bioinorganic chemistry is the application of metal complexes in medicine for diagnostics and therapy of wide range of diseases. The unique properties of the metal complexes and the knowledge about the structure-reactivity-biological activity relationship hold out the opportunity for intelligent design of metallopharmaceuticals with target properties and activity. That is why the subjects in the present teaching course will evolve from the fundamental coordination chemistry knowledge to the direct pharmaceutical applications of metal complexes as therapeutic or diagnostic agents including quickly developing field of radiopharmaceuticals. The students will have the opportunity to synthesize by themselves the first metal-based chemotherapeutics, the cisplatin, during the practical work of this course.</p>										
<p>Requirements for enrollment: NO</p>										

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX050113 ИФ01	Molecular Design	English	BSc	Summer	5	30		30	Prof. A. Tadjer	tadjer@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): Molecular systems with predefined physical and chemical characteristics and/or biological activity are intensively sought both experimentally and theoretically. The course introduces the main classes of materials of interest for modern technologies, cosmetics, and pharmacy. The rules and schemes of QSPR are presented with accent on the design of compounds with potential for utilization into technology, pharmacy, and ecology. During the computational practicum each student is assigned an individual project aimed at modelling of a prospective compound from one of the above-mentioned groups. Specialized software and a wide range of computational methods are applied. The results are discussed and summarized into a term project, which is presented and defended in front of a professional audience at the end of the semester.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦЯ030113 ИН09	Methods for dating of archaeological and geological materials	English	BSc	Winter/ Summer	5	30		30	Assoc. Prof. Petya Kovacheva	nhpk@wmail.chem.uni-sofia.bg

Short description of the course: The course acquaints the students with the methods for absolute and relative dating of different archeological finds (bones, wood, charcoal, ceramics, textile, paper) and geological materials (rocks, minerals, stalactites, stalagmites). Among the methods discussed are: potassium-argon method, radiocarbon, radiocalcium, uranium series, thermoluminescence, fission track method, racemization of aminoacids, isochron dating, dendrochronology, archaeomagnetism, obsidian hydration dating etc. The principle of each method, requirements for sampling, sample preparation and measurement techniques are described. General possibilities and limits of the dating methods are discussed. Examples of dated popular archaeological and geological objects are given to illustrate the applicability of the methods.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX050113 C105	Molecular Modelling of Functional Materials	English	BSc	Summer	5	30		30	Assoc. Prof. G. Madjarova	gmadjarova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course focuses on the application of quantum chemical methods for description of the relationships between the structure and properties of modern functional materials at the molecular level. The lectures introduce students to the mechanisms responsible for the specific characteristics of functional materials and outline the techniques for modelling them theoretically. Using Density Functional Theory, a set of quantities required for assessment of various physical and chemical molecular properties are calculated. The results obtained during the computational practicum for an individually assigned molecule are summarized into a written term project, which is submitted at the end of the semester. The knowledge obtained from the course enables students to perform directed molecular modelling of new more efficient, cheaper, more environmentally friendly, and durable materials.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX050113 ИΦ03	Quantum Chemistry	English	BSc	Winter/ Summer	5	30		30	Prof. A. Tadjer	tadjer@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course acquaints students with the contemporary methods of quantum chemistry and their capacity for application to estimate molecular properties. The methods allowing theoretical determination of molecular characteristics such as geometry, electron density, and energy spectrum are presented. The theoretical foundation and the basic formalism of the methods are summarized and the areas of applicability are discussed. Appropriate illustrative examples are included. Both the lectures and the computational exercises are practically oriented. Each student is assigned an individual term project, which is summarized, submitted in writing and presented orally at the end of the semester. After completing the course students are able to carry out independently a basic computational study of a particular chemical or theoretical problem and to analyse adequately the obtained numerical data using the appropriate specialized software.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX050113 3164	Structure of Matter	English	BSc	Winter	4	45		15	Prof. A. Tadjer Assoc. Prof. G. Madjarova Prof. A. Ivanova	tadjer@chem.uni-sofia.bg gmadjarova@chem.uni-sofia.bg aivanova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course is offered in several versions containing different numbers of academic hours and of ECTS assigned. It encompasses the part of chemistry, which addresses the description of chemical characteristics at the microscopic level. The lectures introduce basic concepts and terms of quantum mechanics and demonstrate their application to chemical objects. The knowledge, which allows prediction of chemical characteristics and theoretical interpretation of the behaviour of real discrete systems is presented. The topics include: energy spectra of atoms and molecules; nature of chemical bonding; molecular structure and electron density; intermolecular forces, hydrogen bonds, modulating effects of the environment, etc. The symmetry apparatus is taught and practiced. During the computational practicum students acquire hands-on experience with basic computational software by using it to calculate molecular properties of an individually assigned molecule. All results are summarized at the end of the semester and presented and discussed during a written test. After completing the course students are familiar with the fundamental concepts of the structure of matter, are able to apply them for interpreting chemical properties at the molecular level, and understand and discuss the outcome of simple molecular simulations.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX050113 ИО09	Optical properties of functional organic compounds	English	BSc	Summer	5	30	30		Assoc. Prof. St. Stoyanov	ohss@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course gives the students an opportunity to expand their knowledge on the fundamental rules which connect the optical properties of organic compounds and their structure. The main approaches towards designed synthesis of organic compounds with desired photophysical properties are discussed along with theoretical and practical training in some of the most powerful “state-of-the-art” spectroscopic techniques and photochemical methods. Special attention will be paid on the reflectance spectroscopy and perception of color, and also on the real-life applications of specific structures for optical sensing, light harvesting, etc. In summary, the course aims at building bridges between the most common spectroscopic methods, the organic compounds’ structure, the fine tuning of their optical properties, and their hi-tech applications.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s’s name	Lecturer/s’s E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX050113 IA08	Modern Instrumental Methods for Analysis - Molecular Spectroscopy and Magnetic Methods	English	BSc /MSc	Summer	5	30		30	Assoc. Prof. Gencheva	ahgg@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The aim of this course is to give a theoretical and practical introduction into selected instrumental analytical methods (UV-Vis and molecular fluorescence spectroscopy, Fourier Transform Infrared (FT-IR) and Raman spectroscopy, circular dichroism, magnetic resonance spectroscopy: NMR and ESR) as well as to present the opportunities for their contemporary application in structural and quantitative characterization of chemicals, bio-molecules and bio-conjugates, polymers, materials, surfaces, etc. The goal of the course is to equip students with practical skills for interpretation of spectra and data and thus to enable them in using of the presented methods in their research work.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s’s name	Lecturer/s’s E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX010113 I02Φ	Quantum Chemistry and Molecular Mechanics	English	BSc	Winter/ Summer	5	45		15	Assoc. Prof. G. Madjarova	gmadjarova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course acquaints students with the modern methods of quantum chemistry and molecular mechanics that allow theoretical determination of molecular characteristics: conformational search, geometry, electronic densities, energy spectrum. The program includes a general introduction of the main classes of modern quantum-chemical methods and discusses their application limits. The potential functions and parameters of the molecular mechanical force field are also discussed. Specific illustrative examples are provided. Lectures and exercises are practically oriented. Each student receives an individual course project.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX010113 И01Φ	Application of Statistics in Molecular Modelling	English	BSc	Summer	5	45		15	Prof. A. Ivanova	aivanova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course enables students to apply basic approaches for statistical analysis to datasets obtained from molecular modelling. The lectures introduce basic concepts of molecular modelling with focus on collection and processing of numerical data yielded by multiple-step molecular simulations. The main goal is presentation of the techniques for statistical analysis of such data arrays. The sources of and methods for estimation of statistical errors are reviewed. The exercises are oriented towards practical mastering of these techniques. Software products for statistical analysis are learned and competences for evaluation of molecular properties by statistical assessment are developed. After completing the course students are able to apply methods for statistical analysis on temporal and other datasets, to extract characteristics of chemical objects and to interpret the physical meaning of the obtained numerical estimates.

Requirements for enrollment: NO

Programme: Bachelor Program Nuclear Chemistry

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		

XФЯ030113 ИА10	Biocoordination chemistry	English	BSc	Summer	5	30		30	Assoc. Prof. A. Ahmedova	ahaa@chem. uni-sofia.bg
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Short description of the course (done in the language of instruction): The modern bioinorganic (biocoordination) chemistry deals with the biological processes involving metalloenzymes and metalloproteins, focusing on the main structural and functional characteristics related to the presence of metal ion(s) in their active site. This involves deeper understanding of the properties of metal ions to form coordination compounds and the corresponding characteristics of their structure and reactivity that are directly connected with the biological activity. Another crucial subject of the bioinorganic chemistry is the application of metal complexes in medicine for diagnostics and therapy of wide range of diseases. The unique properties of the metal complexes and the knowledge about the structure-reactivity-biological activity relationship hold out the opportunity for intelligent design of metallopharmaceuticals with target properties and activity. That is why the subjects in the present teaching course will evolve from the fundamental coordination chemistry knowledge to the direct pharmaceutical applications of metal complexes as therapeutic or diagnostic agents including quickly developing field of radiopharmaceuticals. The students will have the opportunity to synthesize by themselves the first metal-based chemotherapeutics, the cisplatin, during the practical work of this course.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XФЯ030113 ИН09	Methods for dating of archaeological and geological materials	English	BSc	Winter/ Summer	5	30		30	Assoc. Prof. Petya Kovacheva	nhpk@wmail .chem.uni- sofia.bg

Short description of the course: The course acquaints the students with the methods for absolute and relative dating of different archeological finds (bones, wood, charcoal, ceramics, textile, paper) and geological materials (rocks, minerals, stalactites, stalagmites). Among the methods discussed are: potassium-argon method, radiocarbon, radiocalcium, uranium series, thermoluminescence, fission track method, racemization of aminoacids, isochron dating, dendrochronology, archaeomagnetism, obsidian hydration dating etc. The principle of each method, requirements for sampling, sample preparation and measurement techniques are described. General possibilities and limits of the dating methods are discussed. Examples of dated popular archaeological and geological objects are given to illustrate the applicability of the methods.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		

XΦЯ030113 ИФ07	Molecular Design	English	BSc	Summer	5	30		30	Prof. A. Tadjer	tadjer@chem.uni-sofia.bg
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Short description of the course (done in the language of instruction): Molecular systems with predefined physical and chemical characteristics and/or biological activity are intensively sought both experimentally and theoretically. The course introduces the main classes of materials of interest for modern technologies, cosmetics, and pharmacy. The rules and schemes of QSPR are presented with accent on the design of compounds with potential for utilization into technology, pharmacy, and ecology. During the computational practicum each student is assigned an individual project aimed at modelling of a prospective compound from one of the above-mentioned groups. Specialized software and a wide range of computational methods are applied. The results are discussed and summarized into a term project, which is presented and defended in front of a professional audience at the end of the semester.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦЯ030113 ИФ16	Molecular Modelling of Functional Materials	English	BSc	Summer	5	30		30	Assoc. Prof. G. Madjarova	gmadjarova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course focuses on the application of quantum chemical methods for description of the relationships between the structure and properties of modern functional materials at the molecular level. The lectures introduce students to the mechanisms responsible for the specific characteristics of functional materials and outline the techniques for modelling them theoretically. Using Density Functional Theory, a set of quantities required for assessment of various physical and chemical molecular properties are calculated. The results obtained during the computational practicum for an individually assigned molecule are summarized into a written term project, which is submitted at the end of the semester. The knowledge obtained from the course enables students to perform directed molecular modelling of new more efficient, cheaper, more environmentally friendly, and durable materials.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦЯ030113 ИФ09	Quantum Chemistry	English	BSc	Summer	5	30		30	Prof. A. Tadjer	tadjer@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course acquaints students with the contemporary methods of quantum chemistry and their capacity for application to estimate molecular properties. The methods allowing theoretical determination of molecular characteristics such as geometry, electron density, and energy spectrum are presented. The theoretical foundation and the basic formalism of the methods are summarized and the areas of applicability are discussed. Appropriate illustrative examples are included. Both the lectures and the computational exercises are practically oriented. Each student is assigned an individual term project, which is summarized, submitted in writing and presented orally at the end of the semester. After completing the course students are able to carry out independently a basic computational study of a particular chemical or theoretical problem and to analyse adequately the obtained numerical data using the appropriate specialized software.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦЯ030113 3164	Quantum Chemistry and Chemical Bonding	English	BSc	Winter	4	45			Prof. A. Tadjer	tadjer@chem.uni-sofia.bg
									Assoc. Prof. G. Madjarova	gmadjarova@chem.uni-sofia.bg
									Prof. A. Ivanova	aivanova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course provides combined basic knowledge from quantum mechanics and quantum chemistry. The first part is devoted to the basic postulates, approximations, and computational methods for solving Schrödinger's equation. The main classes of quantum chemical methods are summarized. The second part focuses on the theoretical description of specific molecular characteristics and in particular on the nature of chemical bonding in various molecular systems. Symmetry point groups are introduced and the role of symmetry for simplification of selected problems is discussed. Upon completion of the course students are familiar with the basic concepts and methods of quantum chemistry and with the description of the main types of chemical bonds and are able to interpret fundamental properties of atoms and molecules.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦЯ030113 И08А	Radioactive methods in medicine	English	BSc	Winter	4	30	30		Assist. Prof. B. Todorov	B.Todorov@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): Aim of the course is to acquaint students with the use of radioactive isotopes in nuclear medicine and their application for diagnostic and therapeutic radiopharmaceuticals. The basic methods for producing of radioactive isotopes, molecular imaging probes and synthesis of the radiopharmaceuticals are included. Mentioned above methods are discussed with their theoretical bases and examples are given. The lectures are illustrated with practical tasks.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦЯ030113 И009	Optical properties of functional organic compounds	English	BSc	Summer	5	30	30		Assoc. Prof. St. Stoyanov	ohss@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course gives the students an opportunity to expand their knowledge on the fundamental rules which connect the optical properties of organic compounds and their structure. The main approaches towards designed synthesis of organic compounds with desired photophysical properties are discussed along with theoretical and practical training in some of the most powerful "state-of-the-art" spectroscopic techniques and photochemical methods. Special attention will be paid on the reflectance spectroscopy and perception of color, and also on the real-life applications of specific structures for optical sensing, light harvesting, etc. In summary, the course aims at building bridges between the most common spectroscopic methods, the organic compounds' structure, the fine tuning of their optical properties, and their hi-tech applications.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦЯ030113 3236	Organic Chemistry part 2	English	BSc	Winter	7	45	45		Assoc. Prof. St. Stoyanov	ohss@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The aim of the course is to provide students with knowledge on the structure and reactivity of the most important classes of organic compounds. The syllabus for part 2 includes carbonyls, carboxylic acids and their derivatives, amines and amino acids, heterocycles, and natural compounds - carbohydrates, proteins, lipids and nucleic acids. The practicum is divided in laboratory classes and seminars. Laboratory classes aim to train the basic skills required for experimental work in the field of organic chemistry. The seminars help the students to better understand the most important reactions and their mechanisms by means of problem solving and discussions.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦЯ030113 3297	Modern Instrumental Methods for Analysis - Molecular Spectroscopy and Magnetic Methods	English	BSc /MSc	Summer	7	60		30	Assoc. Prof. Gencheva	ahgg@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The aim of this course is to give a theoretical and practical introduction into selected instrumental analytical methods (UV-Vis and molecular fluorescence spectroscopy, Fourier Transform Infrared (FT-IR) and Raman spectroscopy, circular dichroism, magnetic resonance spectroscopy: NMR and ESR) as well as to present the opportunities for their contemporary application in structural and quantitative characterization of chemicals, bio-molecules and bio-conjugates, polymers, materials, surfaces, etc. The goal of the course is to equip students with practical skills for interpretation of spectra and data and thus to enable them in using of the presented methods in their research work.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦЯ030113 IA08	Vibrational Spectroscopy – methods and application	English	BSc	Summer	5	30		30	Assoc. Prof. Gencheva	ahgg@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): In-depth course on the principal of vibrational spectroscopy: Fourier Transform Infrared (FT-IR) spectroscopy, IR-Microscopy, FT-Raman spectroscopy and their use in solving problems of structural, functional and quantitative analysis of organic, organometallic and inorganic compounds.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
XΦX0101 II02Φ	Quantum Chemistry and Molecular Mechanics	English	BSc	Winter/ Summer	5	45		15	Assoc. Prof. G. Madjarova	gmadjarova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course acquaints students with the modern methods of quantum chemistry and molecular mechanics that allow theoretical determination of molecular characteristics: conformational search, geometry, electronic densities, energy spectrum. The program includes a general introduction of the main classes of modern quantum-chemical methods and discusses their application limits. The potential functions and parameters of the molecular mechanical force field are also discussed. Specific illustrative examples are provided. Lectures and exercises are practically oriented. Each student receives an individual course project.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		

XΦX010113 И01Φ	Application of Statistics in Molecular Modelling	English	BSc	Summer	5	45		15	Prof. A. Ivanova	aivanova@chem.uni-sofia.bg
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Short description of the course (done in the language of instruction): The course enables students to apply basic approaches for statistical analysis to datasets obtained from molecular modelling. The lectures introduce basic concepts of molecular modelling with focus on collection and processing of numerical data yielded by multiple-step molecular simulations. The main goal is presentation of the techniques for statistical analysis of such data arrays. The sources of and methods for estimation of statistical errors are reviewed. The exercises are oriented towards practical mastering of these techniques. Software products for statistical analysis are learned and competences for evaluation of molecular properties by statistical assessment are developed. After completing the course students are able to apply methods for statistical analysis on temporal and other datasets, to extract characteristics of chemical objects and to interpret the physical meaning of the obtained numerical estimates.

Requirements for enrollment: NO

Programme: Master program Computational Chemistry

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHC252413 C018	Quantum Chemistry for Molecular Systems	English	MSc	Winter	8	60	45		Prof. A. Tadjer	tadjer@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The main goal of the course is to familiarise the students with the modern quantum chemical methods (Hartree-Fock, post-HF, DFT, etc.). The course is aimed at: introducing the students to the methods allowing theoretical estimation of molecular characteristics – structure, electron density, energy spectra, etc.; serving as background of the solid state theory; laying the basis for the lectures in molecular spectroscopy and hybrid QM/MM methods. The seminars include derivation of some quantum chemical formalistic details. Analytical solving of selected problems is aimed at enabling the students to handle alone specific theoretical problems. Both lectures and seminars are application oriented. Upon completion of the course the students should be able to solve particular scientific problems by means of quantum chemical software packages.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHC252413 C109	Applied Computational Chemistry	English	MSc	Summer	9	30		105	Assoc. Prof. G. Madjarova	gmadjarova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The practicum is set up as a series of theoretical instructions followed by practical assignments aiming at acquainting the students with the tricks and tips in working with professional scientific software in the area of computational chemistry. The topics covered include: preparation of input files; discrimination between versions of the computational procedures; external data sources and import format for non-implemented input; detailed discussion of possible I/O formats; output print options, etc. Various approaches for analysis of molecular characteristics and functions are presented. The advantages and disadvantages of different commercial software packages are outlined and the possibilities for their extension are described. The accumulated skills and the obtained results are presented orally by each student on a weekly basis

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHC252413 C095	Molecular Dynamics and Monte Carlo Simulations	English	MSc	Summer	6	45		30	Prof. A. Ivanova	aivanova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The main goal of the course is to acquaint the students with the theoretical foundation of the two main methods of statistical mechanics, which are applied for molecular modelling of atomic and molecular systems with large number of degrees of freedom. Students should also master practical skills for computational modelling of diverse processes and phenomena from the field of statistical mechanics and thermodynamics and for statistical description of complex systems by classical (atomic and molecular liquids, polymers, micelles, membranes, colloids) and quantum (atoms, spin lattices) methods. Special attention is paid to the methods of analysis of the simulation results, the typical pitfalls of simulating finite-size systems, and the ways of extrapolation of numerical data to physically meaningful macroscopic properties. The course is paralleled by practical exercises, which include typical examples for application of

the methods, students' work with professional program packages, practicing of typical computational techniques and protocols. The purpose is the development of skills for analysis of large numerical arrays and rationalization of theoretical estimates of physical properties.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHC252413 C044	Molecular Mechanics	English	MSc	Winter	5	30		30	Prof. A. Ivanova	aivanova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course introduces the main potential functions for molecular-mechanical (MM) description of molecules. Their use is illustrated by specific examples. The main classes of molecular mechanics force fields for biostructures are presented. The lectures and especially the lab classes are application-oriented.

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHC252413 C025	Quantitative structure-activity relationships (QSARs) of bioactive compounds	English	MSc	Winter	5	30		30	Assoc. Prof. I. Tsakovska	ITsakovska@clbme.bas.bg

Short description of the course (done in the language of instruction): QSAR – quantitative structure-activity relationships - emerged on the basis of advances in quantum chemistry, molecular mechanics, mathematical statistics, and the study of the interaction of molecular ligands and cell receptors. The development of QSAR, on the other hand, became a basis for the appearance of new branches of medicinal chemistry: pharmacophore design, lead structure determination, and docking methods. All these approaches are introduced and their specificities are discussed. The application of these methods leads now to saving huge resources in the development of new drugs and compounds with specific properties. The variety of molecular descriptors employed in 2D QSAR is defined. The most important methods in 3D QSAR are also presented. The key statistical methods employed in QSAR are considered. The course content includes also the basic mechanisms of the interaction between molecular ligands and cell receptors. The laboratory exercises help the students in acquiring practical skills to work with advanced specialized software for QSAR studies.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHC252413 C036	Programming	English	MSc	Winter	6	30		45	Assoc. Prof. V. Tonchev	tonchev@ipc. bas.bg

Short description of the course (done in the language of instruction): The programming language FORTRAN is still preferred for the purposes of scientific programming due to the huge number of existing codes and the tastes of the community. The language and its application for studying various models is the main goal of the course. In view of the orientation of the master degree program basic models, such as the Ising model, random walks, step motions on crystal surfaces, etc., are used throughout the course. The programming language tools and some elementary applications are introduced during the lecture classes, while the practical assignments end with working procedures. Students are expected to write programs alone neglecting the usage of ready-made products. Compilers, translators and debuggers are introduced in the practical assignments. Skills for working with files, finding extrema, working with vectors, matrices, finding eigenvalues spectra, numerical differentiation, numerical integration, numerical solution of ordinary and partial differential equations, and dealing with data from computer experiments are pursued.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHC252413 C064	Modelling of periodic systems and nanostructures	English	MSc / PhD	Summer	4	30		30	Assoc. Prof. H.Aleksandrov	haa@chem.un i-sofia.bg

Short description of the course (done in the language of instruction): The scope of the course is the introduction of the main methods for modelling of periodic systems and nanostructures. The band theory of crystals will be considered for rationalization of the electronic structure. Using the information obtained from the density of states (DOS) and crystal orbital overlap population (COOP), we will analyze how highly delocalized molecular orbitals of solids can be decomposed into the molecular (atomic) orbitals they are constructed of. It will be shown how the concept of interactions between the frontier orbitals can be applied for explanation of properties related to solid state systems and interactions of adsorbates with surfaces. The students will be trained to work with one of the most commonly used program packages for modelling of periodic systems and nanostructures: Vienna Ab initio Simulation Package (VASP). The application of methods and programs for modelling of periodic systems and nanostructures and assessment of their properties will be demonstrated using suitable examples and scenarios.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHC252413 C074	Hybrid (QM/MM) Methods	English	MSc	Summer	4	30		30	Prof. G. Vayssilov	gmv@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The first part of the course describes the necessity of hybrid methods for modelling of complex chemical systems. The isolated cluster approach is also considered and its relevance, features, limitations and applicability are discussed. The next part includes continuum approaches for accounting of the effect of the solvent (environment) on solute molecule. The discrete (atomistic) methods for modelling of complex systems based on combination of quantum chemical and molecular mechanical methods (QM/MM) are presented. The second half of the course is directed towards the application of the hybrid methods to typical examples of complex systems – solutions, different types of organic systems (molecules, transition metal complexes with organic ligands, peptide chains and other biomolecules, etc.), metal oxides, silicates, zeolites. The course includes also exercises and a course project.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHC252413 E034	Introduction to programming in Linux shells and data processing	English	MSc	Summer	4	30		30	Assoc. Prof. P. Petkov	ohpp@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The aim of the course is to introduce the students to shell scripting for Linux. During the course the students will become familiar with the need to write scripts for Linux environments and their use for data processing. The students in computational chemistry usually deal with quantum-chemistry or molecular dynamics calculations. As a result, a large amount of data could be generated. The processing of voluminous data is a time-consuming process that can be automated to facilitate analysis by means of scripts created for specific types of data processing. At the end of the course the students will be able to extract and post-process data from large files and to automate the process of creating input files for quantum chemistry or statistical physics software.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHC252413 E244	Modern Instrumental Methods for Analysis - Molecular Spectroscopy and Magnetic Methods	English	MSc	Summer	4	30		30	Assoc. Prof. Gencheva	ahgg@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The aim of this course is to give a theoretical and practical introduction into selected instrumental analytical methods (UV-Vis and molecular fluorescence spectroscopy, Fourier Transform Infrared (FT-IR) and Raman spectroscopy, circular dichroism, magnetic resonance spectroscopy: NMR and ESR) as well as to present the opportunities for their contemporary application in structural and quantitative characterization of chemicals, bio-molecules and bio-conjugates, polymers, materials, surfaces, etc. The goal of the course is to equip students with practical skills for interpretation of spectra and data and thus to enable them in using of the presented methods in their research work.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHX252413 C084	Computational Methods in Spectroscopy	English	MSc	Summer	4	45		45	Prof. Todor Dudev	t.dudev@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course will acquaint the students with the theoretical methods used as basis for the creation of algorithms and programs for prediction and analysis of molecular spectra. Applications in the three most broadly used spectroscopic methods are included: IR spectroscopy, UV/visible spectroscopy and NMR spectroscopy. The course comprises practical work with various software products used in molecular spectroscopy.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHX252413 C056	Research Practicum	English	MSc	Winter	10			300	All teachers from the Master Programme	aivanova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The practicum is set up as a series of regular (individual, if needed) training activities during which the students will learn how to solve a specific research problem by using theoretical calculations under the guidance of an individual tutor. First, each student is taught how to find information for the particular research problem in specialized portals for scientific journals and/or data bases, how to extract the necessary data thereof, and how to summarize it. Next, the trainees are acquainted with particular functionalities of the software packages, which they need to solve the assigned research task. Then, employing the skills acquired previously in the courses of the M.Sc. programme, the students carry out the planned calculations largely independently. In parallel with that they learn how to organize and discuss numerical results in compliance with the contemporary good scientific practices.

Requirements for enrollment: NO

Programme: Master program Modern Spectral and Chromatographic Analytical Methods

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHX342415 C027	Computational Methods in Spectroscopy	English	MSc	Summer	7	45		45	Prof. Todor Dudev	t.dudev@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course will acquaint the students with the theoretical methods used as basis for the creation of algorithms and programs for prediction and analysis of molecular spectra. Applications in the three most broadly used spectroscopic methods are included: IR spectroscopy, UV/visible spectroscopy and NMR spectroscopy. The course comprises practical work with various software products used in molecular spectroscopy.

Requirements for enrollment: NO										
Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHX342415 C054	Modern Instrumental Methods for Analysis - Molecular Spectroscopy and Magnetic Methods	English	BSc /MSc	Summer	4	30		30	Assoc. Prof. Gencheva	ahgg@chem.uni-sofia.bg
<p>Short description of the course (done in the language of instruction): The aim of this course is to give a theoretical and practical introduction into selected instrumental analytical methods (UV-Vis and molecular fluorescence spectroscopy, Fourier Transform Infrared (FT-IR) and Raman spectroscopy, circular dichroism, magnetic resonance spectroscopy: NMR and ESR) as well as to present the opportunities for their contemporary application in structural and quantitative characterization of chemicals, bio-molecules and bio-conjugates, polymers, materials, surfaces, etc. The goal of the course is to equip students with practical skills for interpretation of spectra and data and thus to enable them in using of the presented methods in their research work.</p>										
Requirements for enrollment: NO										
Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHX342415 E044	Vibrational Spectroscopy – methods and application	English	MSc	Summer	4	30		30	Assoc. Prof. Gencheva	ahgg@chem.uni-sofia.bg
<p>Short description of the course (done in the language of instruction): In-depth course on the principal of vibrational spectroscopy: Fourier Transform Infrared (FT-IR) spectroscopy, IR-Microscopy, FT-Raman spectroscopy and their use in solving problems of structural, functional and quantitative analysis of organic, organometallic and inorganic compounds.</p>										
Requirements for enrollment: NO										

Programme: Master program Pharmacy

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHL382413 E034	Bioinorganic chemistry	English	MSc	Summer/ Winter	4	30		30	Assos. Prof. A. Ahmedova	ahaa@chem.un i-sofia.bg

Short description of the course (done in the language of instruction): The modern bioinorganic (biocoordination) chemistry deals with the biological processes involving metalloenzymes and metalloproteins, focusing on the main structural and functional characteristics related to the presence of metal ion(s) in their active site. This involves deeper understanding of the properties of metal ions to form coordination compounds and the corresponding characteristics of their structure and reactivity that are directly connected with the biological activity. Another crucial subject of the bioinorganic chemistry is the application of metal complexes in medicine for diagnostics and therapy of wide range of diseases. The unique properties of the metal complexes and the knowledge about the structure-reactivity-biological activity relationship hold out the opportunity for intelligent design of metallopharmaceuticals with target properties and activity. That is why the subjects in the present teaching course will evolve from the fundamental coordination chemistry knowledge to the direct pharmaceutical applications of metal complexes as therapeutic or diagnostic agents including quickly developing field of radiopharmaceuticals. The students will have the opportunity to synthesize by themselves the first metal-based chemotherapeutics, the cisplatin, during the practical work of this course.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHL382413 E084	Coordination compounds in medicine	English	MSc	Summer/ Winter	4	30		30	Assos. Prof. A. Ahmedova	ahaa@chem.un i-sofia.bg

Short description of the course (done in the language of instruction): Application of coordination compounds of various metal ions in the contemporary medicine is gaining increasing popularity. Chemotherapy of cancer with platinum complexes is one of the most frequently used methods. Its known shortcomings, however, call for intensive search of more selective and more efficient cytostatics, which is the reason for the rich diversity of novel metal-based antitumour agents as well as the development of new approaches for cancer treatment. The course focuses on the state-of-the-art applications of coordination compounds in therapy and diagnostics along with the prospects to their elaboration. The usage of radiopharmaceuticals for diagnostics and therapy of various diseases is another modern subject that will be presented in this teaching course. The diversity of structures and properties of the metal complexes and the possibility for their fine tuning according to the target application is the key

reason for the broad spectrum of their pharmaceutical application which will be demonstrated with appropriate examples from the nowadays medicinal practice. The knowledge on the properties and the biological role of the essential and toxic metal ions allows for the positive influence on neurodegenerative and cardio-vascular diseases as well as for detoxication through chelation therapy. The students will have the opportunity to synthesize by themselves the first metal-based chemotherapeutics, the cisplatin, during the practical work of this course.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHL382413 C165	Physical Chemistry and Colloid Chemistry 1	English	MSc	Winter	5	30		30	Prof. K. Balashev Prof. A. Ivanova	fhkb@chem.uni-sofia.bg aivanova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The concepts and methods of Physical Chemistry and their application in Pharmacy and Medicine are presented in the course of Physical and Colloid Chemistry. The first general part includes basic approaches: molecular, kinetic and thermodynamic, to describe the properties of homogeneous and heterogeneous single-component and multi-component physicochemical systems. The Laboratory practicum introduces students to some important physicochemical measurements and calculation of molecular properties. Students should acquire fundamental knowledge in the field of Physical Chemistry and use them in subsequent courses for theoretical and experimental characterization of substances and materials with application in pharmacy.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHL382413 E154	Quantitative structure-activity relationships (QSARs) of bioactive compounds	English	MA	Winter	5	30		30	Assoc. Prof. I. Tsakovska	ITsakovska@clbme.bas.bg

Short description of the course (done in the language of instruction): QSAR – quantitative structure-activity relationships - emerged on the basis of advances in quantum chemistry, molecular mechanics, mathematical statistics, and the study of the interaction of molecular ligands and cell

receptors. The development of QSAR, on the other hand, became a basis for the appearance of new branches of medicinal chemistry: pharmacophore design, lead structure determination, and docking methods. All these approaches are introduced and their specificities are discussed. The application of these methods leads now to saving huge resources in the development of new drugs and compounds with specific properties. The variety of molecular descriptors employed in 2D QSAR is defined. The most important methods in 3D QSAR are also presented. The key statistical methods employed in QSAR are considered. The course content includes also the basic mechanisms of the interaction between molecular ligands and cell receptors. The laboratory exercises help the students in acquiring practical skills to work with advanced specialized software for QSAR studies.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHL382413 C418	Pharmaceutical Analysis	English	MA	Summer	8	45		75	Prof. Todor Dudev	t.dudev@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): Students will learn how to apply various analytical techniques (UV/VIS, Fluorescence, Infrared, Raman, Near Infrared, NMR spectroscopy, Mass spectrometry and different chromatographic methods) in studying the structure of the active substance as well as the composition, quality and methods of delivery of vast number of pharmaceutical formulations.

Requirements for enrollment: NO

Course code	Course title (in English)	Language of instruction	Course offered to BA/BS, MA/MS, PhD	Semester	ECTS	Number of hours			Lecturer/s's name	Lecturer/s's E-mail
						Lectures	Exercises/ Seminars	Practical work		
CHL382417 E094	Molecular Modelling of Pharmacophores	English	MSc	Winter	4	30		30	Prof. Anela Ivanova	aivanova@chem.uni-sofia.bg

Short description of the course (done in the language of instruction): The course is designed for all students who want to obtain an overview over methods and techniques applied in computer-assisted pharmacophores design.

Molecular modelling (MM) has seen in the last years a rapid development which reaches far beyond its original goal to easily assess conformation and dynamics of larger molecules essentially provided by molecular mechanics and computer graphics. It has become a powerful tool ranging now from graphical drug design (*de novo* design) to application of neural network and artificial intelligence.

The aim of this course is to present the appropriate tools and basic model for molecular modelling of pharmacophores.

Requirements for enrollment: NO