Course Outline

(1) GENERAL

SCHOOL	SCIENCE		
DEPARTMENT	CHEMISTRY		
DEGREE	MASTER		
COURSE CODE	**18B0**	**SEMESTER**	**3**
COURSE TITLE	Computational Chemistry - Simulation of Properties of Materials with Technological Interest		

INDEPENDENT TEACHING ACTIVITIES in the case that the credits are awarded to separate parts of the course e.g. Lectures, Laboratory Exercises, etc. If the credits are awarded uniformly for the entire course, enter the weekly teaching hours and total credits	**TEACHING HOURS PER WEEK**	**CREDITS**
Lectures	8	10
Add lines if necessary. The teaching organization and methods used are described in detail in (d).		

COURSE TYPE *general background, special background, general knowledge specialization, skill development*	SPECIAL BACKGROUND, GENERAL KNOWLEDGE SPECIALIZATION, SKILL DEVELOPMENT
PREREQUISITE COURSES:	NO
COURSE AND EXAM LANGUAGE:	GREEK
IS THE COURSE OFFERED TO ERASMUS STUDENTS ?	IF NEEDED YES
COURSE WEBSITE (URL)	https://eclass.uoa.gr/courses/CHEM258/

(2) LEARNING OUTCOMES

LEARNING OUTCOMES

The learning outcomes, specific knowledge, skills and abilities of an appropriate level that the students will acquire after the successful completion of the course are described.

Consult Appendix A

• Description of the Level of Learning Outcomes for each course of study according to the Qualifications Framework of the European Higher Education Area

• Descriptive Indicators for Levels 6, 7 & 8 of the European Qualifications Framework for Lifelong Learning and Annex B

• Comprehensive Guide to writing Learning Outcomes

The main objective of this course is to get acquainted with the computational methods using for solving problems of the science of chemistry.

During the course the following tasks are discussed,

- Various computational methods based on the theory of molecular orbitals (ab-initio) and on Electrons' Density Functionals (DFT).
- Applications to problems concerning materials with technological interest.
- Computational chemistry packages (Gaussian, MOPAC, etc.) and their capabilities.

Knowledge

- Knowledge and understanding of the basic principles of molecular orbitals and Electron's density functionals' theoretical methods.
- Knowledge and understanding of the use of the Computational chemistry packages (Gaussian, MOPAC, etc.) and their capabilities.
- Knowledge and understanding of the prediction of chemical activity based on structural characteristics of chemical species (symmetry, bond strength, molecular valence orbitals, etc.), their electrical properties (atomic charges, electronegativity, etc.).
- Knowledge and understanding of the intermolecular interactions.

Skills

- Skills in evaluating basic results of computational chemistry studies.
- Skills in designing and using appropriate structural models for studying long-range interactions in chemical systems.
- Skills in analyzing the molecular structures and relating these to their properties.
- Skills in using molecular design programs and measuring the structural features and properties of molecules.
- Skills in the literature search of original and review articles in the field of computational chemistry.

Abilities

- Ability to apply the knowledge gained by the students in dealing with problems related to computational chemistry.

- Ability to interpret calculated data from the ab-initio and/or DFT studies of molecular and periodic chemical systems and relate them to their structural, spectroscopic, and electric properties.
- Ability to evaluate the local structure of crystalline and amorphous materials, surfaces, nanomaterials, etc.
- Ability to predict and/or analyze the electronic transitions, vibrational and NMR spectra, the effect of the presence of a solvent, and the interaction (strong or weak) between the molecules.
- Ability to calculate the electrical properties like dipole moment, polarizability, the atomic charges and electrostatic surface.

General Skills

Taking into account the general skills that the graduate must have acquired (as stated in the Diploma Appendix and listed below) which of the following is/are the course aimed at?.

Reearch, analysis and synthesis of data and information, using the necessary technologies	*Project planning and management*
Adaptation to new situations	*Respect for diversity and multiculturalism*
Decision making	*Respect for the environment*
Independent work	*Demonstrating social, professional and ethical responsibility and sensitivity to gender issues*
Teamwork	*Exercise criticism and self-criticism*
Working in an international environment	*Promotion of free, creative and inductive thinking*
Working in an interdisciplinary environment	*Other…….*
Generating new research ideas	

The course aims at equipping students with the following general skills:

- Search, analysis and synthesis of data and information, using the necessary technologies.
- Autonomous work.
- Group work.
- Ability to apply knowledge to problem solving.
- Generation of new research ideas.
- Work in an interdisciplinary environment.
- Promotion of free, creative, and inductive thinking.
- Decision making.

(3) COURSE CONTENT

Various methods based on the theory of molecular orbitals (ab-initio) and on Electrons' Density Functionals (DFT) as well as their application to problems concerning materials with technological applications. Computational chemistry packages (Gaussian, MOPAC, etc.) and their capabilities.
Practice on the computer on,
Total molecular energy calculation problems and optimization of the molecular systems' structure, techniques for studying the local structure of crystalline and amorphous materials, surfaces, nanomaterials, etc., the effect of the presence of a solvent, the interaction (strong or weak) between the molecules, calculation of the electrical properties like dipole moment, polarizability, etc., calculation of the atomic charges and electrostatic surface, simulation of the electronic transitions, vibrational and NMR spectra.
The above calculated properties will be linked to the research projects (Diploma Theses) of students.

(4) TEACHING AND LEARNING METHODS – EVALUATION

<table>
<tr><td>LECTURES' DELIVERY
In person, distance, etc..</td><td>In person</td></tr>
<tr><td>USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGIES
Use of I.C. T. in Lectures, Laboratory Exercises, Communication with students</td><td>In Teaching:
Presentations with multimedia content (power point).
Practical courses using computational chemistry software.
In Communication with students:
Support the learning process through the e-class electronic platform (announcements, information, messages, documents, user groups, etc.).
Email.</td></tr>
<tr><td>TEACHING ORGANIZATION
The teaching style and methods are described in detail.
Lectures, Seminars, Laboratory Exercises, Field Exercises, Literature Study & Analysis, Tutorial, Internship (Placement), Clinical Exercises, Art Workshop, Interactive Teaching, Educational Visits, Study Preparation (Project), PaperWriting Assignments, Artistic Creation, etc. etc.

The student's study hours for each learning activity as well as unguided study hours according to ECTS principles are listed</td><td><table><tr><th>Activity</th><th>Semester workload</th></tr><tr><td>Lectures</td><td>78</td></tr><tr><td>Unguided study</td><td>62</td></tr><tr><td>Paper writing</td><td>50</td></tr><tr><td>Projects' preparation</td><td>30</td></tr><tr><td>Meetings</td><td>10</td></tr><tr><td>Study preparation</td><td>20</td></tr><tr><td>total</td><td>250</td></tr></table></td></tr>
<tr><td>STUDENT EVALUATION
Description of the evaluation process

Assessment Language, Assessment Methods, Formative or Deductive, Multiple Choice Test, Short Answer Questions, Essay Development Questions, Problem Solving, Written Assignment, Report / Report, Oral Examination, Public Presentation, Laboratory Work, Clinical Patient Examination, Artistic Interpretation, Other / Others

Explicitly defined evaluation criteria are mentioned, and if and where they are accessible by students.</td><td>The evaluation of the course takes place in Greek and includes:
Computational study of the structural, electric, and vibrational properties of a specific molecular system.
Projects.</td></tr>
</table>

(5) RECOMMENDED BIBLIOGRAPHY

- Introduction to Computational Chemistry, Second Edition, Frank Jensen, John Wiley & Sons Inc., ISBN-13: 978-0-470-01186-7.
- Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems. David C. Young, Copyright (2001 John Wiley & Sons, Inc. ISBNs: 0-471-33368-9 (Hardback); 0-471-22065-5 (Electronic).

- Essentials of Computational Chemistry, Theories and Models, Second Edition, Christopher J. Cramer, John Wiley & Sons Ltd, ISBN 0-470-09181-9.