COURSE OUTLINE

(1) GENERAL

SCHOOL	SCHOOL OF SCIENCES		
DEPARTMENT	DEPARTMENT OF CHEMISTRY		
LEVEL OF STUDIES	ISCED level 6 – Bachelor's or equivalent level		
COURSE CODE	YN401	**SEMESTER**	4th Semester
COURSE TITLE	Physical Chemistry II		

TEACHING ACTIVITIES *If the ECTS Credits are distributed in distinct parts of the course e.g. lectures, labs etc. If the ECTS Credits are awarded to the whole course, then please indicate the teaching hours per week and the corresponding ECTS Credits.*	**TEACHING HOURS PER WEEK**	**ECTS CREDITS**
	4 Th +3 Lab	7
Please, add lines if necessary. Teaching methods and organization of the course are described in section 4.		

COURSE TYPE *Background, General Knowledge, Scientific Area, Skill Development*	General Background
PREREQUISITES:	
TEACHING & EXAMINATION LANGUAGE:	Greek
COURSE OFFERED TO ERASMUS STUDENTS:	NO
COURSE URL:	https://eclass2.emt.duth.gr/courses/CHEM_D104/

(2) LEARNING OUTCOMES

Learning Outcomes
Please describe the learning outcomes of the course: Knowledge, skills and abilities acquired after the successful completion of the course.

Upon successful completion of the course, the student will have acquired fundamental knowledge regarding the quantum behavior of matter and be able to interpret spectroscopic measurements and observations. Furthermore, the student will be capable of addressing problems using statistical thermodynamics methods and studying the kinetics of chemical reactions.
The main objectives of the Laboratory are:
a) to familiarize students with large-scale research infrastructure,
b) to provide training in laboratory techniques and foster the acquisition of experimental skills, and
c) to consolidate knowledge of Physical Chemistry by bridging theory and experiment.
Upon successful completion of the laboratory course, students will be able to:

- Understand physicochemical processes related to surface physical chemistry and the physicochemical properties of fluids
- Master the process of preparing laboratory reports, including performing physicochemical calculations and generating diagrams to derive the required physicochemical parameters
- Process and present the results of experimental exercises effectively
- Demonstrate knowledge and understanding of fundamental concepts, principles, and theories related to the fields of surface science and the physicochemical properties of fluids
- Understand the applications of material characterization methods
- Utilize data from international scientific literature
- Employ appropriate experimental methods or a combination of methods to solve complex Physical Chemistry problems

- Apply complex problem-solving skills by analyzing data from international literature
- Apply their knowledge to address problems related to electrochemistry, surface physical chemistry, and the physicochemical properties of fluids
- Collaborate effectively with fellow students or researchers on topics involving electrochemistry, surface physical chemistry, and the physicochemical properties of fluids
- Work efficiently both as part of a team and autonomously
- Operate within an international environment

Training in the Physical Chemistry Laboratory is designed to cultivate critical thinking and a scientific mindset. It reinforces initiative and active learning, while simultaneously developing team spirit and cooperation through group laboratory practice

General Skills

Name the desirable general skills upon successful completion of the module

Search, analysis and synthesis of data and information,
ICT Use
Adaptation to new situations
Decision making
Autonomous work
Teamwork
Working in an international environment
Working in an interdisciplinary environment
Production of new research ideas
Project design and management
Equity and Inclusion
Respect for the natural environment
Sustainability
Demonstration of social, professional and moral responsibility and sensitivity to gender issues
Critical thinking
Promoting free, creative and inductive reasoning

Working in an interdisciplinary environment
Generating new research ideas
Respect for the natural environment
Exercising criticism and self-criticism
Promoting free, creative, and inductive thinking

The general skills acquired by students and targeted by the laboratory course are:

- Theoretical thinking and the ability to convert theoretical knowledge into solving and finding experimental parameters
- The ability to apply knowledge acquired during their studies in related courses of the Department's PPE
- Ability to search for, analyze, and synthesize data and information from the international literature and use the necessary technologies related to the presentation of research results
- Acquisition of the appropriate practical knowledge background to enable further education at the postgraduate level
- Working in an interdisciplinary environment
- Ability to collaborate at the team level to achieve the above objectives

(3) COURSE CONTENT

THEORY

1. **Principles of Quantum Mechanics.** Electromagnetic radiation, blackbody radiation, photoelectric effect, Compton effect, Bohr theory, wave-particle duality of matter. Schrödinger equation. The Born interpretation of the wavefunction.
2. **Techniques and Applications of Quantum Theory.** Transportation motion. Vibrational motion. Rotational motion.
3. **Atomic Structure and Atomic Spectra.** Structure and spectra of hydrogenic atoms. Structure of polyelectronic atoms. Slater determinant. Pauli exclusion principle. Spectra of complex atoms.
4. **Introduction to Molecular Quantum Chemistry.** The Born-Oppenheimer approximation. Valence-bond theory. Molecular orbital theory. Molecular orbitals for polyatomic systems.
5. **Molecular Symmetry.** Elements of group theory. Applications of symmetry in molecular orbital theory – Polyatomic molecules. Localized molecular orbital theory. Hybridization. Computational techniques in Quantum Chemistry. The Hückel approximation and prediction of molecular properties.
6. **Statistical Thermodynamics.** The distribution of molecular states. Internal energy and entropy. The canonical partition function. Independent molecules.

7. **Applications of Statistical Thermodynamics.** Average energies, heat capacities, equilibrium constants. Statistical properties of Macromolecules – Colloids.
8. **Molecular Interactions.** Electric properties of molecules. Polarizability. Polarization. Intermolecular interactions. Molecular interactions in gases. The liquid-vapor interface. Surface films. Condensation.
9. **Molecular Motion in Gases.** Molecular motion in liquids. Diffusion.
10. **Chemical Reaction Rates.** Experimental rate law. Reaction order and integrated rate laws. Temperature dependence and the Arrhenius equation. Determination of reaction mechanism from the rate law. Elementary reactions. Consecutive reactions. Examples of reaction mechanisms. Photochemistry.
11. **Reaction Dynamics.** Reactive encounters. Collision theory. Transition state theory.

LABORATORY

1. Langmuir-Blodgett Film Deposition Method (LB).
2. Determination of surface tension of solutions – Wilhelmy plate method.
3. Determination of interfacial tension – Spinning drop method (for liquid-liquid interfacial tensions).
4. Determination of contact angle during liquid-solid-gas interface interaction (Contact Angle Analyzer [CA]).
5. Material microstructure characterization methods I: Mercury Porosimetry (Mercury Porosimeter).
6. Material microstructure characterization methods II: Nitrogen Porosimetry – BET method (Nitrogen Porosimeter).
7. Atomic Force Microscopy (Atomic Force Microscope [AFM]).
8. Scanning Electron Microscopy: Familiarization with the operation of the electron microscope and X-ray analyzer (Scanning Electron Microscope with EDS (X-ray spectrometry) [SEM-EDX]).

(4) LEARNING & TEACHING METHODS - EVALUATION

<table>
<tr><td>TEACHING METHOD
Face to face, Distance learning, etc.</td><td>Lectures on the board
Face-to-face tutorials and laboratory exercises</td></tr>
<tr><td>USE OF INFORMATION & COMMUNICATIONS TECHNOLOGY (ICT)
Use of ICT in Teaching, in Laboratory Education, in Communication with students</td><td>THEORY
Use of ICT (Power point) in Teaching
More than 200 multiple-choice questions using the click questions method (based on the MIT model).
LABORATORY
Use of ICT (PowerPoint and video) in teaching. Support for the learning process through the e-class electronic platform. Specifically, the slides from the tutorials, the theory and experimental instructions are posted, the pre-lab test is conducted, and the lab reports are submitted.
Communication with students via email, answering questions.</td></tr>
<tr><td>TEACHING ORGANIZATION
The ways and methods of teaching are described in detail.
Lectures, Seminars, Laboratory Exercise, Field Exercise, Bibliographic research & analysis, Tutoring, Internship (Placement), Clinical Exercise, Art Workshop, Interactive learning, Study visits, Study / creation, project, creation, project. Etc.

The supervised and unsupervised workload per activity is indicated here, so that total workload per semester complies to ECTS standards.</td><td>
<table>
<tr><th>Activity</th><th>Workload/semester</th></tr>
<tr><td>Lectures and problems (4 hours x 13 weeks)
Laboratory exercises (3 hours per week x 13 weeks)</td><td>91</td></tr>
<tr><td>Final exam (3 hours)</td><td>3</td></tr>
<tr><td>Student study hours, preparation for progress and final exam</td><td>81</td></tr>
<tr><td>Total Course Hours
25 hours per credit</td><td>175
Total workload</td></tr>
</table>
</td></tr>
<tr><td>STUDENT EVALUATION
Description of the evaluation process</td><td>Student evaluation methods
Written final exam on Theory</td></tr>
</table>

Assessment Language, Assessment Methods, Formative or Concluding, Multiple Choice Test, Short Answer Questions, Essay Development Questions, Problem Solving, Written Assignment, Essay / Report, Oral Exam, Presentation in audience, Laboratory Report, Clinical examination of a patient, Artistic interpretation, Other/Others *Please indicate all relevant information about the course assessment and how students are informed*	Minimum passing grade: 5 The lab grade is determined by the following: i. Careful and successful execution of experiments—Lab participation, grade A1, 5% ii. The lab notebook, which includes the presentation and evaluation of the experimental results and questions to reinforce the material, grade A2, 25% iii. The midterm written exam on the material covered in the laboratory exercises (progress), grade B1, 35% iv. The final written exam on the material covered in the laboratory exercises, grade B2, 35% The final overall grade for the course "Physical Chemistry Laboratory I" is calculated as follows: Final grade = {A1}x0.05 + {A2}x0.25 + {B1}x0.35 + {B2}x0.35 At the end of each semester, there is a week of make-up laboratory exercises. Students who have been absent once (1) during the current semester are eligible to participate. If a student has more than one absence, they must repeat the missed laboratory experiments in the following academic year. Students who have been absent from more than four laboratory exercises (≥4) must re-register for the course in a future semester and repeat all experiments. Successful completion of all laboratory experiments is a prerequisite for students to take the final written exam. If a student has completed the laboratory part of the exercises but has a laboratory grade lower than 5, they are given the opportunity to participate in a partial laboratory exam in September. The final overall grade for the course is calculated as follows: Final grade = {Theory}x0.60 + {Laboratory}x0.40

(5) SUGGESTED BIBLIOGRAPHY

- Προτεινόμενη Βιβλιογραφία:

1. P. Atkins, J. De Paula, Φυσικοχημεία, Πανεπιστημιακές εκδόσεις Κρήτης (2015).
2. D.A. McQuarrie, Quantum Chemistry, Univ. Sci. Books (1983).
3. C.J. Cramer, Computational Chemistry, Wiley (2004).
4. Δ. Α. Γιαννακουδάκη, Μαθήματα Θερμοδυναμικής και Φ. Χημείας, Θεσ/νικη (1975).
5. Ν. Κατσάνος, Φυσικοχημεία: βασική θεώρηση, εκδόσεις Παπαζήση (1998).
6. W.J. Moore, Physical Chemistry, Longmans 4th ed. London (1962).
7. I.N. Levine Physical Chemistry, 6th ed., Mc Graw Hill, New York (2009).
8. L.C. Labowitz, J.S. Arents, Problems in Physical Chemistry Khosla Pub. (1995).
9. David R. Lide, CRC Handbook of Chemistry and Physics, 84th Ed., 2003-2004
10. Α. Γιαννακουδάκης, Μ. Σιγάλας, Π.Γιαννακουδάκης, Υβριδικές Εργαστηριακές Ασκήσεις σε θέματα Φυσικής Χημείας, Εκδόσεις Τζιόλα

- Συναφή επιστημονικά περιοδικά:

1. Journal of Chemical Education

The Physics Teacher