

# COURSE OUTLINES

## 1<sup>st</sup> Semester

### Advanced Topics in Physical Chemistry and in Statistical Thermodynamics of Materials

#### COURSE OUTLINE

#### 1. GENERAL

SCHOOL	NATURAL SCIENCES		
ACADEMIC UNIT	DEPARTMENT OF MATERIALS SCIENCE		
PARTICIPATING INSTITUTIONS			
POSTGRADUATE PROGRAMME: TITLE OF POSTGRADUATE PROGRAMME	MATERIALS SCIENCE		
LEVEL OF STUDIES	7 <sup>th</sup> (Master of Science Degree)		
COURSE CODE	EY_A1	SEMESTER	1 <sup>st</sup>
COURSE TITLE	Advanced Topics in Physical Chemistry and in Statistical Thermodynamics of Materials		
<b>INDEPENDENT TEACHING ACTIVITIES</b>	<b>WEEKLY TEACHING HOURS</b>	<b>CREDITS</b>	
	3	10	
COURSE TYPE	General background		
PREREQUISITE COURSES:	None		
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek (English if needed)		
IS THE COURSE OFFERED TO ERASMUS STUDENTS	Yes		
COURSE WEBSITE (URL)	<a href="https://www.matersci.upatras.gr/images/joomlart/university/docs/PMS/Msc_Materials_Science_Sintomos_Odigos.pdf">https://www.matersci.upatras.gr/images/joomlart/university/docs/PMS/Msc_Materials_Science_Sintomos_Odigos.pdf</a>		

#### 2. LEARNING OUTCOMES

Learning outcomes
Based on the principles of statistical mechanics, quantum mechanics, and thermodynamics, physicochemical phenomena of central importance for the design of materials and the understanding of the structure-property relationship are studied. Topics include phase transitions, molecular self-organization and self-assembly, polymers and soft materials, transport phenomena, diffusion, Langevin equation, electrons in metals - Fermi gas, and phonons in crystals. The course, according to the European Qualifications Framework for Lifelong Learning, is at level 7 as a postgraduate program.
General Competences
Search for, analysis and synthesis of data and information, Working independently, Team work, Production of new research ideas, Production of free, creative and inductive thinking

### 3. SYLLABUS

Review of the basic principles of thermodynamics. Classical and quantum description of microstates of atomic and molecular systems. Probability distributions, correlation functions and connection with statistical mechanics. Statistical ensembles and their equivalence in the thermodynamic limit. Applications: statistical mechanics of polymer chains, response of paramagnetic and dielectric materials to weak static external fields.

Spontaneous magnetization, Ising model in one dimension, Bragg-Williams approximation, Bethe-Peierls approximation, equivalence of the Ising model with other models (Lattice gas, Binary alloy), Landau theory of free energy, continuous phase transitions, critical exponents, Van der Waals gas.

Quantum statistics. Density of states. Fermions and bosons. Free electron model (Fermi gas model), Fermi energy and heat capacity calculation. Einstein and Debye model for phonons and calculation of heat capacity. Photon statistics and description of light-matter interaction according to Einstein.

Transport phenomena. Derivation of diffusion equation, thermal conductivity equation, and viscosity, in one and three spatial dimensions. Systems with production or dissipation of energy/particles/momentum. Examples of thermal conductivity and diffusion. Biased diffusion, Einstein relation. Applications of diffusion in drug delivery. Langevin equation and Brownian motion. Linear response, correlation functions, fluctuation-dissipation theorem.

### 4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY.	Face-to-face		
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY	Teaching includes use of ICT as well as whiteboard for in depth presentation of theory and problem solving		
TEACHING METHODS	<b>Activity</b>	<b>Semester workload</b>	
	lectures	39	
	Home work	100	
	Study and analysis of bibliography	111	
	Course total	<b>250</b>	
STUDENT PERFORMANCE EVALUATION	<p>Problem solving during written final exam.</p> <p style="text-align: center;"><b>General criteria for the assessment of students</b></p> <p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course.</p>		

### 5. RECOMMENDED BIBLIOGRAPHY

- 1) *Thermodynamics and an Introduction to Thermostatistics, 2<sup>nd</sup> Ed.*, Herbert B. Callen, Wiley (1985)
- 2) *Statistical and Thermal Physics: With Computer Applications*, H. Gould and J. Tobochnik, Princeton University Press (2010)
- 3) *Introduction to Phase Transitions and Critical Phenomena*, H. Stanley, Oxford University Press (1987)
- 4) *Statistical Mechanics, 2<sup>nd</sup> Ed.*, Kerson Huang, Wiley (1987)

5) *Introduction to Statistical Physics, 2<sup>nd</sup> Ed.*, Kerson Huang, CRC Press (2010)

6) *An Introduction to Statistical Mechanics and Thermodynamics, 2<sup>nd</sup> Ed.*, Robert H. Swendsen, Oxford University Press (2020).

7) *Basic chemical thermodynamics, 5<sup>th</sup> Ed.*, E. Brian Smith, Imperial College Press (2004)

8) *A modern course in statistical physics, 4<sup>th</sup> Ed.*, Linda E. Reichl, Wiley-VCH (2016)

9) *Molecular driving forces: Statistical Thermodynamics in Biology, Chemistry, Physics, and Nanoscience, 2<sup>nd</sup> Ed.*, Ken A. Dill and Sabrina Bromberg, Taylor & Francis (2011)

10) *Concepts in Thermal Physics*, S. J. Blundell and K. M. Blundell, Oxford University Press (2010)

11) *Atkins' Physical Chemistry*, P. Atkins and J. De Paula, 8<sup>th</sup> Ed. Oxford University Press (2006)

12) *Fundamentals and Applications of Controlled Release Drug Delivery*, Eds. Siepmann, Siegel, and Rathbone, Springer (2012)

# Advanced Experimental Techniques for Materials Characterization

## COURSE OUTLINE

### 1. GENERAL

SCHOOL	NATURAL SCIENCES		
ACADEMIC UNIT/PARTICIPATING UNITS	MATERIALS SCIENCE		
PARTICIPATING INSTITUTIONS			
POSTGRADUATE PROGRAMME: TITLE OF POSTGRADUATE PROGRAMME	Materials Science		
LEVEL OF STUDIES	Postgraduate		
COURSE CODE	EY-A2	SEMESTER	1 <sup>st</sup>
COURSE TITLE	Advanced Experimental Techniques for Materials Characterization		
INDEPENDENT TEACHING ACTIVITIES	WEEKLY TEACHING HOURS	CREDITS	
	3	10	
COURSE TYPE	Specialised general knowledge		
PREREQUISITE COURSES:	NO		
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek or English if it is required		
IS THE COURSE OFFERED TO ERASMUS STUDENTS	YES		
COURSE WEBSITE (URL)	<a href="https://eclass.upatras.gr/courses/MSCI623/">https://eclass.upatras.gr/courses/MSCI623/</a>		

### 2. LEARNING OUTCOMES

Learning outcomes
With the successful completion of the course students will be able to identify which advanced characterization technique should choose depending on the type of behaviour/properties of the materials should be determined. They will know the general principles of the theoretical background of the characterization techniques described in the current syllabus. Students will be able to know the principles of operation of the characterization techniques, and the methodology of acquiring and analyzing experimental data.
General Competences
<ul style="list-style-type: none"> <li>- Search for, analysis and synthesis of data and information, with the use of the necessary technology</li> <li>- Adapting to new situations</li> <li>- Working independently</li> <li>- Team work</li> <li>- Working in an international environment</li> <li>- Working in an interdisciplinary environment</li> <li>- Production of new research ideas</li> <li>- Project planning and management</li> <li>- Respect for the natural environment</li> <li>- Criticism and self-criticism</li> <li>- Production of free, creative and inductive thinking.</li> </ul>

### 3. SYLLABUS

X-Ray Diffraction. X-rays in the electromagnetic radiation spectrum, production of x-rays, Bragg's Law, the X-ray Diffractometer and what information it provides, structure determination, grain-size evaluation from Scherrer formula, the Vegard's Law and the determination of stoichiometry of solid solutions, determination of thin film thickness and multilayer periodicity.

Optical Microscopy. Principles of geometrical and physical optics. The optical System. The compound optical microscope. Abbe theory and imaging resolution. Apertures, field stop diaphragms and illumination. Dark field, phase contrast, polarization and interferometric microscopy systems. Technical elements and specifications.

Spectroscopic techniques for the characterization of carbon nanostructured materials and metallic nanoparticles. Study of graphene and related materials, carbon nanotubes, metal nanoparticles and other nanomaterials with Raman, FTIR, UV-Vis, luminescence spectroscopy, thermogravimetry, X-ray diffraction and X-ray photoelectron spectroscopy etc.

Scanning Electron Microscopy (SEM): Instrumentation, beam-sample interactions, backscattered electrons, secondary electrons, detectors, Energy dispersive X-Ray spectrometry (EDAX), sample preparation, applications.

Dielectric spectroscopy. Response of non-conductive materials to electric field. Types of dielectric materials. Influence of direct and alternating field on the electrical properties of materials. Complex dielectric permittivity, real and imaginary part of dielectric permittivity. Formalism for analyzing the electrical behaviour of non-conductive materials. Dielectric relaxations in materials. AC conductivity. Experimental methodology and methods for analyzing data.

Dynamic mechanical thermal analysis. Introduction to thermal processes, materials response under varying stresses or strains. Creep, stress relaxation. Storage modulus, loss modulus, loss tangent (damping factor). Mechanical relaxations in materials. Experimental methodology and methods for analyzing data.

Optical spectroscopy/Laser Raman Spectroscopy. Radiation-matter interaction and Light-scattering spectroscopies. This module has a duration of six hours (two 3-hour lectures). The aim is to introduce students to basic concepts of radiation-matter interaction. Initially, there is an introduction to the characteristics of various types of radiation and their technological significance. This is followed by correlating radiation characteristics with the discrete energy levels of molecules. The concepts of absorption, emission, and scattering are defined, with an emphasis on the basic elements of Rayleigh scattering. The fundamental elements of vibrational spectroscopy, and in particular Raman scattering, are developed. Reference is made to polarization geometries as well as to the method of analyzing polarized spectra from crystalline and amorphous materials. The basic elements of Raman scattering instrumentation are presented, with emphasis on laser sources, as well as signal collection, analysis, and recording systems. Finally, special aspects of Raman spectroscopy are presented, specifically surface-enhanced techniques and Fourier-transform Raman spectroscopy.

Electrochemical methods for the characterization of materials, cyclic voltammetry (CV), linear sweep voltammetry (LSV), square wave voltammetry (SWV), differential pulse voltammetry (DPV), chronoamperometry (CA) and spectroelectrochemistry.

Introduction to Scanning Tunneling Microscopy. Introduction to Atomic Force Microscopy. A Short History of Scanning Probe Microscopy. Scanning Probe Microscopy Instrumentation (Transients of Oscillations Dissipation and Quality Factor of a Damped Driven Harmonic Oscillator). Technical Aspects of Scanning Probe Microscopy (Piezoelectric Effect Extensions of Piezoelectric Actuators Piezoelectric Materials Tube Piezo Element Resonance Frequencies of Piezo Tubes Non-linearities and Hysteresis Effects of Piezoelectric Actuators, Thermal Drift, STM Tip Preparation, Vibration Isolation, Isolation of the Microscope from Outer Vibrations, Combining Vibration Isolation and a Microscope with High Resonance Frequency). Scanning Probe Microscopy Designs. Electronics for Scanning Probe Microscopy. Artifacts in SPM (Tip-Related Artifacts). Work Function, Contact Potential, and Kelvin Probe Scanning Force Microscopy (Work Function, Effect of a Surface on the Work Function, Surface Charges and External Electric Fields, Contact Potential Measurement of Work Function by the Kelvin Method, Kelvin Probe Scanning Force Microscopy). Surface States (Surface States in a One-Dimensional Crystal, Surface States in 3D Crystals, Surface States Within the Tight Binding Model, Atomic Force Microscopy (Forces Between Tip and Sample, Tip-Sample Forces, Snap-to-Contact). Technical

Aspects of Atomic Force Microscopy (Requirements for Force Sensors, Fabrication of Cantilevers, Beam Deflection Atomic Force Microscopy, Sensitivity of the Beam Deflection Method, Detection Limit of the Beam Deflection Method). Principles of Static Atomic Force Microscopy. Friction Force Microscopy (FFM). Amplitude Modulation (AM)

Mode in Dynamic Atomic Force Microscopy. Intermittent Contact Mode/Tapping Mode (Atomic Force Microscopy with Large Oscillation. Frequency Modulation (FM) Mode in Dynamic Atomic Force Microscopy—Non-contact Atomic Force Microscopy. Noise in Atomic Force Microscopy (Thermal Noise Density of a Harmonic Oscillator and its application in the Static/Dynamic AFM mode).

Thermal analysis. Thermogravimetry (TG), Differential Thermal Analysis (DTA), Differential Scanning Calorimetry (DSC), Triple Core Differential Scanning Calorimetry, Differential scanning calorimetry with regenerative power, Temperature modulated Differential Scanning Calorimetry, Kissinger plot. Applications of thermal analysis in the study of amorphous metallic glasses

#### 4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY.	Face-to-face	
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY	Teaching of the course is carried out via weekly lectures with slides via a video projector, where the theory is thoroughly analysed and the methodology of the experiments and the methods of data analysing is presented. Students are conducting lab experiments, write lab reports and present their results.	
TEACHING METHODS	<i>Activity</i>	<i>Semester workload</i>
	Lectures	39
	Studying-Literature research	160
	Laboratory exercises	10
	Writing experimental reports/project presentation	41
	Course total	<b>250</b>
STUDENT PERFORMANCE EVALUATION	<p>The final evolution is the result of: (i) a Written examination at the end of the semester, (ii) the experimental reports/presentations (each one contributes up to 10%). The total rate of contribution to the final grade of the experimental reports/presentations cannot exceed the 50% of final grade.</p> <p style="text-align: center;"><b>General criteria for the assessment of students</b></p> <p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course.</p>	

#### 5. RECOMMENDED BIBLIOGRAPHY

*- Suggested bibliography:*

Thermal analysis of polymers, fundamentals and applications, J. D. Menczel, R. B. Prime, Wiley 2009.

Springer Handbook of Materials Measurements Methods, H. Czichos, T. Saito, L. Smith, Springer 2006.

Conductivity and dielectric characterization of polymer nanocomposites, G. C. Psarras, p. 31-69, in "Polymer nanocomposites: Physical properties and applications", edited by S. C. Tjong and Y.-M. Mai, ISBN: 978-1-84569-6726. Woodhead Publishing Limited, Cambridge, 2010.

*- Related academic journals:*

Journal of materials Science, Express Polymer Letters, Journal of Polymer Science: Part B: Polymer Physics, Materials Chemistry and Physics, Journal of Thermal Analysis and Calorimetry.

# Micro and Nano-phase Materials and Nanoscience

## (Devices and Functionalities)

### COURSE OUTLINE

#### 1. GENERAL

SCHOOL	NATURAL SCIENCES		
ACADEMIC UNIT/PARTICIPATING UNITS	MATERIALS SCIENCE		
PARTICIPATING INSTITUTIONS			
POSTGRADUATE PROGRAMME: TITLE OF POSTGRADUATE PROGRAMME	Materials Science		
LEVEL OF STUDIES	Postgraduate		
COURSE CODE	EY-A4	SEMESTER	2 <sup>nd</sup>
COURSE TITLE	Micro and Nano-phase Materials and Nanoscience (Devices and Functionalities)		
INDEPENDENT TEACHING ACTIVITIES	WEEKLY TEACHING HOURS	CREDITS	
	3	10	
COURSE TYPE	Specialised general knowledge		
PREREQUISITE COURSES:	NO		
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek or English if it is required		
IS THE COURSE OFFERED TO ERASMUS STUDENTS	YES		
COURSE WEBSITE (URL)	<a href="https://www.matersci.upatras.gr/el/studies/postgraduate/epistimi-ton-ylikon/msccourses">https://www.matersci.upatras.gr/el/studies/postgraduate/epistimi-ton-ylikon/msccourses</a>		

#### 2. LEARNING OUTCOMES

Learning outcomes
<p>The student should acquire the following learning outcomes after the successful completion of the course:</p> <ul style="list-style-type: none"> <li>- Understands and knows selected categories of micro- and nano-materials, their functionality and the corresponding devices for applications of high interest</li> <li>- Understands and knows the optical and electronic properties of semiconductor nanomaterials- excitons/biexcitons</li> <li>- He has special knowledge on the calculation of optical energy gaps using quantum mechanical models</li> <li>- Understands and knows the physical fabrication methods of semiconductor nanomaterials as well as characterization methods</li> <li>- Has specific knowledge of electrode materials and electrochemical energy storage devices (eg lithium ion batteries, supercapacitors).</li> <li>- Understands and knows basic physicochemical and electrochemical characteristics of energy storage devices.</li> </ul>

- Possesses highly specialized knowledge, some of which is cutting-edge knowledge in a field of work or study and which forms the basis for original thinking.
- Knows how to search and collect scientific information.
- Possesses a critical awareness of knowledge issues in a field and its interaction with other fields.
- Writes a scientific text
- Has become familiar with the oral presentation of scientific papers. They are able to communicate with clarity their conclusions as well as the knowledge and background on which they are based together with the logical assumptions employed, both to specialized and non-specialized audience.

The course is characterized as Level 7 course of second-cycle studies, according to the European Qualifications Framework for Lifelong Learning

#### General Competences

- Search for, analysis and synthesis of data and information, with the use of the necessary technology - Adapting to new situations
- Working independently
- Team work
- Working in an international environment
- Working in an interdisciplinary environment
- Production of new research ideas
- Project planning and management
- Respect for the natural environment
- Criticism and self-criticism
- Production of free, creative and inductive thinking

### 3. SYLLABUS

Introduction to methods and procedures for the synthesis and development of nano/microphase materials as well as single nanoparticles. The physicochemical properties of nanoparticles and the role of the presence of micro/nano structures in the macroscopic properties of materials are described. The basic principles of nanotechnology are introduced for the design of materials based on the desired properties and the construction of their devices. Types of nanoparticles, preparation and characterization methods. Electronic, magnetic, optical, chemical, mechanical properties at the nanoscale. Low dimensional systems quantum dots, nanowires, semiconductors. Nanomaterials for energy storage

### 4. TEACHING and LEARNING METHODS - EVALUATION

<b>DELIVERY.</b>	Face-to-face	
<b>USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY</b>	Teaching of the course is carried out via weekly lectures with slides via a video projector, where the theory is thoroughly analysed and the methodology of writing a bibliographic work is presented. Students present their work through slides	
<b>TEACHING METHODS</b>	<i>Activity</i>	<i>Semester workload</i>
	Lectures	80
	Study-Search of Bibliography	90
	Discussion-Bibliography analysis	50
	Preparation of bibliographic work and presentation	30

	Course total	250
STUDENT PERFORMANCE EVALUATION	<p>The evaluation procedure is a combination of:</p> <p>(a) short-answer questions</p> <p>(b) oral examination</p>	
	<p>(c) bibliographic work</p> <p>(d) presentation of bibliographic work</p> <p>The language of evaluation is Greek or English</p> <p style="text-align: center;"><b>General criteria for the assessment of students</b></p> <p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course.</p>	

## 5. RECOMMENDED BIBLIOGRAPHY

### - **Suggested bibliography:**

"Electrochemical Devices for Energy Storage Applications", Ed. M.A. Kebede & F.I. Ezema, CRC Press, 2019.

"Carbon Nanomaterials for Electrochemical Energy Technologies. Fundamentals and Applications", Edited by S. Sun, X. Sun, Z. Chen, Y. Liu, CRC Press, 2017.

"Quantum Wells, Wires and Dots, Theoretical and Computational Physics of Semiconductor Nanostructures", Paul Harrison, Alex Valavanis, Wiley

"The Physics of Low-dimensional Semiconductors, An Introduction", John H. Davies, Cambridge University Press

"The Physics of Semiconductors, An Introduction including Nanophysics and Applications", Third Edition, Marius Grundmann, Springer

"Optical Properties of Solids", Second Edition, Mark Fox, Oxford University Press.

### - **Related academic journals:**

Journal of Power Sources, Batteries, ASC Nano, ACS Applied materials & Interfaces, Applied Energy, Chemical Engineering Journal, ACS Applied Nanomaterials, Nanomaterials, Journal of Materials Science

# Materials modelling

## COURSE OUTLINE

### 1. GENERAL

SCHOOL	NATURAL SCIENCES		
ACADEMIC UNIT	DEPARTMENT OF MATERIALS SCIENCE		
PARTICIPATING INSTITUTIONS			
POSTGRADUATE PROGRAMME: TITLE OF POSTGRADUATE PROGRAMME	MATERIALS SCIENCE		
LEVEL OF STUDIES	7 <sup>th</sup> (Master Degree)		
COURSE CODE	EY_A5	SEMESTER	1 <sup>st</sup>
COURSE TITLE	Materials modelling		
INDEPENDENT TEACHING ACTIVITIES		WEEKLY TEACHING HOURS	CREDITS
		3	10
COURSE TYPE	General background		
PREREQUISITE COURSES:	None		
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek (English if needed)		
IS THE COURSE OFFERED TO ERASMUS STUDENTS	yes		
COURSE WEBSITE (URL)	<a href="https://www.matersci.upatras.gr/images/joomlart/university/docs/PMS/Msc_Materials_Science_Sintomos_Odigos.pdf">https://www.matersci.upatras.gr/images/joomlart/university/docs/PMS/Msc_Materials_Science_Sintomos_Odigos.pdf</a>		

### 2. LEARNING OUTCOMES

Learning outcomes
<p>Introduction to basic physical models from mechanics, electromagnetism, and quantum mechanics used in the Science of Materials. Introduction to fundamental simulation methods for materials ranging from atomic to macroscale. Understanding the capabilities and limitations of models and theoretical/computational methods for studying and predicting material properties and parameters. The course, according to the European Qualifications Framework for Lifelong Learning, is at level 7 as a postgraduate program.</p>
General Competences
<p>Search for, analysis and synthesis of data and information, Working independently, Team work, Production of new research ideas, Production of free, creative and inductive thinking</p>

### 3. SYLLABUS

In the course we initially present continuum models and the problem of coupled harmonic oscillators and use them for the modelling of mechanical and optical properties of materials. We then present a unified treatment of wave propagation in electronic and electromagnetic material systems and introduce the essentials of the transfer matrix method, a powerful analytical tool that can be used to model and study an array of problems pertaining to wave

propagation in electrons and photons. We also present the power computational method of Finite-Difference TimeDomain (FDTD) method and use commercial package (ANSYS FDTD) or/and open-source code (ANGORA) for its implementation. The transfer matrix and FDTD methods are then applied to quantum materials including quantum nanostructures, as well as photonic materials and structures, like periodic photonic structures, plasmonics, lasers, and others. We also present the tight-binding approach to electronic structure calculations, Time-dependent density functional calculations, Plane wave density functional calculations, and Molecular dynamics.

#### 4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY.	Face-to-face	
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY	Teaching includes use of ICT as well as whiteboard for in depth presentation of theory and problem solving	
TEACHING METHODS	<b>Activity</b>	<b>Semester workload</b>
	lectures	39
	Course assignments	70
	Study and analysis of bibliography	61
	Semester project	80
	Course total	<b>250</b>
STUDENT PERFORMANCE EVALUATION	<p>Evaluation with semester project and assignments during the course.</p> <p style="text-align: center;"><b>General criteria for the assessment of students</b></p> <p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course.</p>	

#### 5. RECOMMENDED BIBLIOGRAPHY

- 13) *Computational Nanoscience*, Kalman Varga and Joseph A. Driscoll, Cambridge University Press (2011)
- 14) *Computer Simulations of Liquids, 2<sup>nd</sup> Ed.*, Michael P. Allen and Dominic J. Tildesley, Oxford University Press (2017)
- 15) *Numerical Electromagnetics: The FDTD method*, Umran S. Inan and Robert A. Marshall, Cambridge University Press (2011)
- 16) *Computational Electrodynamics (The Finite-Difference Time-Domain Method), 3<sup>rd</sup> Ed.*, A. Taflove, Artech House Publishers (2005)
- 17) *Wave Propagation: From Electrons to Photonic Crystals and Left-Handed Materials*, P.Markos and C.M. Soukoulis, Princeton University Press (2008)
- 18) *ANGORA: A Free Software Package for Finite-Difference Time-Domain Electromagnetic Simulations*, I. Capoglu, A. Taflove, and V. Backman, IEEE Antennas and Propagation Magazine 55(4), 81 (2013)

## 2<sup>nd</sup> Semester

### Direction A'

## Advanced Materials: Design, Synthesis and Processing

### COURSE OUTLINE

#### 1. GENERAL

SCHOOL	NATURAL SCIENCES		
ACADEMIC UNIT/PARTICIPATING UNITS	MATERIALS SCIENCE		
PARTICIPATING INSTITUTIONS			
POSTGRADUATE PROGRAMME: TITLE OF POSTGRADUATE PROGRAMME	Materials Science		
LEVEL OF STUDIES	Postgraduate		
COURSE CODE	EY_B1.1	SEMESTER	2 <sup>nd</sup>
COURSE TITLE	Advanced Materials: Design, Synthesis and Processing		
INDEPENDENT TEACHING ACTIVITIES	WEEKLY TEACHING HOURS	CREDITS	
	3	7	
COURSE TYPE	Specialised general knowledge		
PREREQUISITE COURSES:	NO		
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek or English if it is required		
IS THE COURSE OFFERED TO ERASMUS STUDENTS	YES		
COURSE WEBSITE (URL)	<a href="https://www.matersci.upatras.gr/el/studies/postgraduate/epistimi-ton-ylikon/msccourses">https://www.matersci.upatras.gr/el/studies/postgraduate/epistimi-ton-ylikon/msccourses</a>		

#### 2. LEARNING OUTCOMES

Learning outcomes
The student should acquire the following learning outcomes after the successful completion of the course: <ul style="list-style-type: none"><li>- Understands and knows selected categories of advanced materials, such as biomimetic materials, metal alloys and monolithic catalytic materials and reactors.</li><li>- Understands the physicochemical processes of materials of interest.</li><li>- He has special knowledge on selected catalytic processes of environmental and energy interest</li></ul>

- Possesses highly specialized knowledge, some of which is cutting-edge knowledge in a field of work or study and which forms the basis for original thinking.
- Knows how to search and collect scientific information.
- Possesses a critical awareness of knowledge issues in a field and its interaction with other fields.
- Writes a scientific text
- Has become familiar with the oral presentation of scientific papers. They are able to communicate with clarity their conclusions as well as the knowledge and background on which they are based together with the logical assumptions employed, both to specialized and non-specialized audience.

The course is characterized as Level 7 course of second-cycle studies, according to the European Qualifications Framework for Lifelong Learning

#### General Competences

- Search for, analysis and synthesis of data and information, with the use of the necessary technology - Adapting to new situations
- Working independently
- Team work
- Working in an international environment
- Working in an interdisciplinary environment
- Production of new research ideas
- Project planning and management
- Respect for the natural environment
- Criticism and self-criticism
- Production of free, creative and inductive thinking

### 3. SYLLABUS

Design, synthesis and processing refer to the development and use of processes that result in the controlled arrangement of atoms, molecules and molecular aggregates in appropriate configurations to produce the desired behavior, depending on the application. These processes aim to control the structure and properties of materials at all levels, from the atomic to the macroscopic level. An introduction is made to selected categories of advanced materials such as biomimetic materials, metal alloys and monolithic catalytic materials and devices of high environmental and energy interest.

### 4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY	Face-to-face	
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY	Teaching of the course is carried out via weekly lectures with slides via a video projector, where the theory is thoroughly analyzed and the methodology of writing a bibliographic work is presented. Students present their work through slides	
TEACHING METHODS	<i>Activity</i>	<i>Semester workload</i>
	Lectures	60
	Study-Search of Bibliography	70
	Discussion-Bibliography analysis	30
	Preparation of bibliographic work and presentation	15
	Course total	<b>175</b>

STUDENT PERFORMANCE EVALUATION	<p>The evaluation procedure is a combination of:</p> <ul style="list-style-type: none"> <li>(e) short-answer questions</li> <li>(f) oral examination</li> <li>(g) bibliographic work</li> <li>(h) presentation of bibliographic work</li> </ul>
	<p>The language of evaluation is Greek or English</p> <p style="text-align: center;"><b>General criteria for the assessment of students</b></p> <p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course.</p>

#### 5. RECOMMENDED BIBLIOGRAPHY

**- Suggested bibliography:**

“Heterogeneous Catalysis: Fundamentals and Applications” (J.R.H. Ross, Editor), Elsevier B.V., Amsterdam, 2012

“Elements of Chemical Reaction Engineering” (H. Scott Fogler), by K. Filippopoulos & G Marnellos, Ed., Tziola Publications, 5th Edition, 2018

“Catalytic Reactors” by Basudeb Volkan Saha Degirmenci (Editor), Walter de Gruyter, 2015

“Επιστήμη και Τεχνολογία των Μεταλλικών Υλικών», Γ. Χρυσουλάκης, Δ. Παντέλης, Εκδ. Παπασωτηρίου, 2η εκδ. 2007.

**- Related academic journals:**

ASC Nano, ACS Applied materials & Interfaces, Applied Catalysis B, Chemical Engineering Journal, ACS Applied Nanomaterials, Nanomaterials, Green Chemistry, Surface and Interfaces, Journal of Materials Science, Nanoscale

# Micro/Nano-technology of Materials

## COURSE OUTLINE

### 1. GENERAL

SCHOOL	NATURAL SCIENCES		
ACADEMIC UNIT	DEPARTMENT OF MATERIALS SCIENCE		
PARTICIPATING INSTITUTIONS			
POSTGRADUATE PROGRAMME: TITLE OF POSTGRADUATE PROGRAMME	MATERIALS SCIENCE		
LEVEL OF STUDIES	7 <sup>th</sup> (Master Degree)		
COURSE CODE	EY_B2.1	SEMESTER	2 <sup>nd</sup>
COURSE TITLE	Micro/Nano-technology of Materials		
<b>INDEPENDENT TEACHING ACTIVITIES</b>	<b>WEEKLY TEACHING HOURS</b>	<b>CREDITS</b>	
	3	7	
COURSE TYPE	General background		
PREREQUISITE COURSES:	NO		
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek/English if needed		
IS THE COURSE OFFERED TO ERASMUS STUDENTS	yes		
COURSE WEBSITE (URL)	<a href="https://www.matersci.upatras.gr/images/joomlart/university/docs/PMS/Msc_Materials_Science_Sintomos_Odigos.pdf">https://www.matersci.upatras.gr/images/joomlart/university/docs/PMS/Msc_Materials_Science_Sintomos_Odigos.pdf</a>		

### 2. LEARNING OUTCOMES

Learning outcomes
In-depth introduction and deep insight to materials of micro- and nano-metric dimensions as well as the examination of the phenomena that arise from the limitation of the active materials' parts in systems of such low dimensions. Theoretical methods for the study of the properties of the materials, preparation of various micro- and nano-metric material type and classes, examples of such materials and devices as well as related technological applications that are promising in various areas, such as for example. in the construction of integrated Circuits, storage of energy, microscopy, mechanics and others. The course, according to the European Qualifications Framework for Lifelong Learning, is at level 7 as a postgraduate program
General Competences
Search for, analysis and synthesis of data and information, Working independently, Team work, Production of new research ideas, Production of free, creative and inductive thinking

### 3. SYLLABUS

--

In-depth introduction and deep insight to materials of micro- and nano-metric dimensions as well as the examination of the phenomena that arise from the limitation of the active materials' parts in systems of such low dimensions.

Theoretical methods for the study of the properties of the materials, preparation of various micro- and nano-metric material type and classes, examples of such materials and devices as well as related technological applications that are promising in various areas, such as for example. in the construction of integrated Circuits, storage of energy, microscopy, mechanics and others.

Specifically:

Schrödinger Wave Equation. Particle in Quantum Well, Quantum Well, Wire and Dot, Scattering and Tunneling in 1D, Applications of Tunneling, Energy Bands in Solids, Bloch Wavefunction and the Kronig-Penney Potential, E - k Dispersion and Energy Bands.

Quantum Treatment of Harmonic Oscillator: the algebraic method. Schrödinger Treatment of central potentials. A spherical potential well. Hydrogen Atom, Angular Momentum Operators, Spherical Harmonics and Spatial Quantization.

Perturbation Theory, Time-Independent Perturbation Theory for non-degenerate and degenerate states. Time-Dependent Perturbation Theory, Harmonic Perturbation and Fermi's Golden Rule, System of Identical Particles and Electron Spin, Electron Spin, Interaction of Electron Spin with Magnetic Field, Electron Paramagnetic Resonance.

Atom-Field Interaction, Atom-Field Interaction: Semi-Classical Treatment, Driven Two Level Atom, Atom-Field Interaction: Quantum Treatment, The Interaction of Electromagnetic Waves with Resonant Optical Media, Atomic Susceptibility, Attenuation and Amplification of Light.

Ionic Bond and Van der Waals Attraction (Polyatomic Molecules and Hybridized Orbitals, Molecular Spectra, Theoretical Background, Rotational and Vibrational Spectra of Diatomic Molecule, Nuclear Spin and Hyperfine Interaction, Nuclear Magnetic Resonance (NMR).

Carrier Transport in Semiconductors (Quantum Description of Transport Coefficients, Equilibrium and NonEquilibrium, Generation and Recombination Currents).

P-N Junction Diode: I-V Behavior and Device Physics (The p-n Junction in Equilibrium, The p-n Junction under Bias, Ideal Diode I-V Behavior, Non-Ideal I-V Behavior, P-N Junction Diode: Applications, Optical Absorption, Photodiode, Solar Cell, LED and LD, Field Effect Transistors, The Modeling of MOSFET I-V, Silicon Nanowire Field Effect Transistor, Tunneling NWFET as Low Power Device, The Application and Novel Kinds of FETs, Non-Volatile flash EEPROM Cell, Semiconductor Solar Cells, Biosensor, Spin Field Effect Transistor, Spin Qubits and Quantum Computing),

Fundamentals of Micro/Nanoscale Electronic Devices (Design, Electronic/optical/magnetic properties, experimental methods towards design and manufacturing, relation to the active materials' properties).

#### 4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY	Face-to-face		
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY	Teaching includes use of ICT as well as whiteboard for in depth presentation of theory and problem solving		
TEACHING METHODS	<b>Activity</b>	<b>Semester workload</b>	
	lectures	39	
	Home work	100	

	Study and analysis of bibliography	111
	Course total	<b>250</b>

STUDENT PERFORMANCE EVALUATION	<p>Problem solving during written final exam.</p> <p style="text-align: center;"><b>General criteria for the assessment of students</b></p> <p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course.</p>
--------------------------------	--

#### 5. RECOMMENDED BIBLIOGRAPHY

*Martin-Palma R. J. and Martinez-Duart J. M., Nanotechnology for Microelectronics and Photonics, 2<sup>nd</sup> edition, 2017*

*Gaponenko, S. V. Introduction to Nanophotonics. 2010. <https://doi.org/10.1017/cbo9780511750502>.*

*Natelson, D. Nanostructures and Nanotechnology. 2015. <https://doi.org/10.1017/cbo9781139025485>.*

*Akkermans, E.; Gilles Montambaux. Mesoscopic Physics of Electrons and Photons. 2007. <https://doi.org/10.1017/cbo9780511618833>.*

*Haus, J. W. Fundamentals and Applications of Nanophotonics. 2016. <https://doi.org/10.1016/c2014-0-01442-6>.*

*Mitin V. et al.. Introduction to Nanoelectronics; 2007. <https://doi.org/10.1017/cbo9780511809095>.*

*Kim, Dae Mann. Introductory Quantum Mechanics for Applied Nanotechnology; 2015. Steel, D. G., Introduction to Quantum Nanotechnology: A Problem Focused Approach, 2022*

# Master Thesis I

## COURSE OUTLINE 1.

### GENERAL

SCHOOL	NATURAL SCIENCES		
ACADEMIC UNIT/PARTICIPATING UNITS	MATERIALS SCIENCE		
PARTICIPATING INSTITUTIONS			
POSTGRADUATE PROGRAMME: TITLE OF POSTGRADUATE PROGRAMME	Materials Science		
LEVEL OF STUDIES	Postgraduate		
COURSE CODE	EY-MT1.1	SEMESTER	2 <sup>nd</sup>
COURSE TITLE	Master Thesis I		
INDEPENDENT TEACHING ACTIVITIES		WEEKLY TEACHING HOURS	CREDITS
		-	10
COURSE TYPE	Specialised general knowledge		
PREREQUISITE COURSES:	NO		
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek or English if it is required		
IS THE COURSE OFFERED TO ERASMUS STUDENTS	YES		
COURSE WEBSITE (URL)	-		

### 2. LEARNING OUTCOMES

Learning outcomes
Conducting Master Thesis I. In the first part of the Thesis is conducted bibliographic survey of the subject. The subject of the Thesis is determined in collaboration with the Supervising Professor.
General Competences
<ul style="list-style-type: none"> <li>- Search for, analysis and synthesis of data and information, with the use of the necessary technology - Adapting to new situations</li> <li>- Working independently</li> <li>- Team work</li> <li>- Working in an international environment</li> <li>- Working in an interdisciplinary environment</li> <li>- Production of new research ideas</li> <li>- Project planning and management</li> <li>- Respect for the natural environment</li> <li>- Criticism and self-criticism</li> <li>- Production of free, creative and inductive thinking</li> </ul>

### 3. SYLLABUS

Bibliographic survey of the Thesis's subject.
---

#### 4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY.	Face-to-face		
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY	Using electronic (web) tools for literature search.		
TEACHING METHODS	<i>Activity</i>	<i>Semester workload</i>	
	Studying-Literature research	100	
	Writing bibliographic essays reports/project presentation	150	
	<b>Course total</b>	<b>250</b>	
STUDENT PERFORMANCE EVALUATION	<p>Students are evaluated via the conducted bibliographic survey and the writing of the theoretical part of their Thesis.</p> <p style="text-align: center;"><b>General criteria for the assessment of students</b></p> <p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course.</p>		

#### 5. RECOMMENDED BIBLIOGRAPHY

- *Suggested bibliography:*  
 Because of the nature of the course, specific bibliography cannot be recommended. - *Related academic journals:*

**Biomaterials, Biomolecular and Biomimetic Systems**  
**(STRUCTURE, INTERACTIONS, BIOCOMPATIBILITY AND BIOTECHNOLOGY)**  
 COURSE OUTLINE 1.

GENERAL

SCHOOL	NATURAL SCIENCES		
ACADEMIC UNIT/PARTICIPATING UNITS	MATERIALS SCIENCE		
PARTICIPATING INSTITUTIONS			
POSTGRADUATE PROGRAMME: TITLE OF POSTGRADUATE PROGRAMME	MATERIALS SCIENCE		
LEVEL OF STUDIES	POSTGRADUATE		
COURSE CODE	EY_B3.1	SEMESTER	2 <sup>nd</sup>
COURSE TITLE	BIOMATERIALS, BIOMOLECULAR AND BIOMIMETIC SYSTEMS (STRUCTURE, INTERACTIONS, BIOCOMPATIBILITY AND BIOTECHNOLOGY)		
INDEPENDENT TEACHING ACTIVITIES		WEEKLY TEACHING HOURS	CREDITS
Teaching		2	6
COURSE TYPE	Specialised general knowledge		
PREREQUISITE COURSES:	NO		
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	GREEK (English if needed)		
IS THE COURSE OFFERED TO ERASMUS STUDENTS	YES		
COURSE WEBSITE (URL)	<a href="https://www.matersci.upatras.gr/el/studies/postgraduate/epistimi-ton-ylikon/msscourses">https://www.matersci.upatras.gr/el/studies/postgraduate/epistimi-ton-ylikon/msscourses</a>		

2. LEARNING OUTCOMES

Learning outcomes
<p>At the end of this course the student should be able to:</p> <p>Have a complete understanding of the structure and organization of biological molecular species in materials.</p> <p>Have acquired highly specialized knowledge, some of which is cutting-edge knowledge in the field of work or study related to the science of biomaterials and biomolecular systems. Also, to have a critical knowledge in the above field and its interconnection with different fields.</p> <p>Have specialized problem-solving skills required in research and/or innovation to develop new knowledge and processes and to integrate knowledge from different fields.</p> <p>Have the knowledge that will assist them in the professional approach to their work or profession and have competencies that are typically proved by developing and supporting logical arguments and problem solving in the context of Materials Science.</p>
General Competences

Search for, analysis and synthesis of data and information  
 Adapting to new situations  
 Working independently

Team work  
 Working in an international environment  
 Working in an interdisciplinary environment  
 Project planning and management  
 Production of free, creative and inductive thinking

### 3. SYLLABUS

The understanding of the structure and organization of biological molecular species in materials. Next, the mechanism of formation and organization of important materials such as teeth and bones are explored, and the structure-properties relationship for each material is also studied. This knowledge is crucial to enable the student to evaluate the advantages and disadvantages of using biobased materials as biomaterials and to design new materials based on the unique and peculiar structures of biomaterials.

### 4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY.	Face to face	
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY	Lectures using power point presentation as well as demonstration experiments in the class.	
TEACHING METHODS	<i>Activity</i>	<i>Semester workload</i>
	Lectures	26
	Homework and Projects	124
	Course total	150
STUDENT PERFORMANCE EVALUATION	<p>The evaluation of the students is done by written final semester examination (in Greek) which includes:</p> <ol style="list-style-type: none"> <li>1. Short answer questions</li> <li>2. Development of topics</li> </ol> <p>In addition, is given the possibility of presenting small projects whose degree is counted in the final grade.          Students have the right to view their exam scripts after grading.</p> <p style="text-align: center;"><b>General criteria for the assessment of students</b></p> <p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course.</p>	

### 5. RECOMMENDED BIBLIOGRAPHY

1. K. N. Demetzos «Modern Pharmaceutical Technology», Parisianos Editions. 2022
2. Mikos, Antonios G., Temenoff, Johnna S., «Biomaterials: The interface between materials science and biology» Utopia Editions, 2017

*Related academic journals:*

1. Biomaterials

2. Acta Biomaterialia

3. Journal of Biomedical Materials Research - Part B Applied Biomaterials

# Molecular Materials

## COURSE OUTLINE

### 1. GENERAL

SCHOOL	NATURAL SCIENCES		
ACADEMIC UNIT	DEPARTMENT OF MATERIALS SCIENCE		
PARTICIPATING INSTITUTIONS			
POSTGRADUATE PROGRAMME: TITLE OF POSTGRADUATE PROGRAMME	MATERIALS SCIENCE		
LEVEL OF STUDIES	7 <sup>th</sup> (Master Degree)		
COURSE CODE	EY_B4.1	SEMESTER	2 <sup>nd</sup>
COURSE TITLE	MOLECULAR MATERIALS		
<b>INDEPENDENT TEACHING ACTIVITIES</b>	<b>WEEKLY TEACHING HOURS</b>	<b>CREDITS</b>	
	3	6	
COURSE TYPE	General background		
PREREQUISITE COURSES:	Successful completion of A semester		
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek/English if needed		
IS THE COURSE OFFERED TO ERASMUS STUDENTS	yes		
COURSE WEBSITE (URL)	<a href="https://www.matersci.upatras.gr/images/joomla/university/docs/PMS/Msc_Materials_Science_Sintomos_Odigos.pdf">https://www.matersci.upatras.gr/images/joomla/university/docs/PMS/Msc_Materials_Science_Sintomos_Odigos.pdf</a>		

### 2. LEARNING OUTCOMES

Learning outcomes
<p>Understanding the basic concepts related to molecular structure, molecular interactions, self-organization and selfbuilding and their importance in determining the properties of molecular materials and devices that are of modern interest: colloidal systems, dendrimers, nanomagnets, pure polymers, carbon nanostructures, hybrid organic inorganic semiconductors (perovskites).</p> <p>The course, according to the European Qualifications Framework for Lifelong Learning, is at level 7 as a postgraduate program.</p>
General Competences
Search for, analysis and synthesis of data and information, Working independently, Team work, Production of new research ideas, Production of free, creative and inductive thinking

### 3. SYLLABUS

--

Understanding the basic concepts related to molecular structure, molecular interactions, self-organization and selfbuilding and their importance in determining the properties of molecular materials and devices that are of modern interest: colloidal systems, dendrimers, nanomagnets, pure polymers, carbon nanostructures, hybrid organic inorganic semiconductors (perovskites).

Specifically:

Introduction to Molecular Materials

The Versatility of Molecular Chemistry

Top-Down and Bottom-Up Approaches

Guide to Design Functional Molecular Materials(Basic Concepts of Magnetism,Magnetochemistry, and Molecular Magnetism,Magnetic Field,Magnetic Induction,Magnetic Moment,Effect of Magnetic Field on Matter,Magnetization,Magnetic permeability and,susceptibility,Electronic Magnetic Moments,Classical model of magnetic,moments,Quantum mechanical model,of magnetic moments,Magnetic Properties of Free Atoms, ,The Curie Law,The Curie–Weiss Law,Deviations from the Curie Law,Effective Magnetic Moment and  $\chi T$  Value,Field Dependence of Magnetization,Magnetic Exchange Coupling,Magnetic Exchange Coupling in a Dinuclear Compound,Multicenter Magnetic Systems and,Spin Hamiltonian Approach)

Transport Properties of Molecular Materials(Electrical Conductivity,Classes of Conducting Materials,Energy Bands and Origin of Transport Properties,Thermal Dependence of Conductivity,Types of Semiconducting Materials,Band Theory of Solids,Structural Anisotropy and Peierls Distortion)

Principles of Molecular Photophysics(Electromagnetic Radiation and Light–Matter Interaction,Electronic Energy States,Electronic, rotational, and vibrational states,Absorption of radiation,Transition moment integral and selection rules,The Franck–Condon principle,Evolution of Excited States,Luminescence,Kasha’s rule,Fluorescence and phosphorescence,Luminescent and nonluminescent molecules,Jablonski diagram,Emission Efficiency,Quantum yield and luminescence quenching,Kinetics of photophysical processes,Emission lifetime,Dynamics of radiative decay,Energy Transfer,Dexter’s energy transfer,Förster’s energy transfer,Quenching,Dynamic and static quenching,Metal-Centered Electronic Transitions,d–d transitions,f-f transitions)

Magnetic Molecular Materials (Paramagnetism, Ferromagnetism, Antiferromagnetism, Ferrimagnetism, Spin Crossover, Valence Tautomerism, Slow Magnetic Relaxation, Single-molecule magnets, Single-ion magnets, Single-chain magnets, Molecular spin qubits)

Conducting Molecular Materials (Charge Transfer Salts, Radical Cation Salts, Radical Anion Salts, Single-Component Molecular, Conductors,Chiral Molecular Conductors, Enhanced conductivity in enantiopure chiral conductors, Electrical magnetochiral anisotropy)

Optical Molecular Materials(Electronic Transitions and Light, Absorption in Metal Complexes, Structural/optical properties relationship, Energy, Intensity, Luminophores with a Structural Role of the Metal, Effect of the metal, Effect of the ligand, Supramolecular effects, Luminophores Based on Open-Shell, d-Metal Complexes, First-row transition metal complexes, Second- and third-row transition metal complexes, Luminophores Based on Lanthanide Complexes, Ligand-to-metal sensitization, Sensitized lanthanide emission, Molecular NLOphores, SHG NLOphores)

Multifunctional Molecular Materials(A Family of Paramagnetic Superconductors, Magnetic-Field-Induced Superconductivity in a Paramagnetic Metal, Ferromagnetic Metal-Like Conductors, Coexistence of Electrical Conductivity and Slow Magnetic Relaxation in a Hybrid Material, Synergism between Electrical Conductivity and SpinCrossover Behavior, A Molecular Ferromagnet with an Increased Coercive Field, Optical Control in a Chiral Photomagnet, Multiemissive Molecular Materials, Superimposed Optical Properties, Cooperative Optical Properties)

Conducting Luminescent Materials (Turning Molecular Materials into Devices, Organic Light-Emitting Diodes, Optical Fibers and Amplifiers for Telecommunication, Dye-Sensitized Solar Cells, Single-Molecule Magnets)

Special cases to be discussed for materials also characterized as colloidal systems, dendrimers, molecular nanomagnets, conducting polymers, nanostructures carbon and finally as hybrid organic inorganic semiconductors (perovskites).

#### 4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY.	Face-to-face		
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY	Teaching includes use of ICT as well as whiteboard for in depth presentation of theory and problem solving.		
TEACHING METHODS	<b>Activity</b>	<b>Semester workload</b>	
	lectures	39	
	Home work	60	
	Study and analysis of bibliography	51	
	Course total	<b>150</b>	
STUDENT PERFORMANCE EVALUATION	<p>Problem solving during written final exam.</p> <p style="text-align: center;"><b>General criteria for the assessment of students</b></p> <p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course.</p>		

#### 5. RECOMMENDED BIBLIOGRAPHY

- Anderson, P. W. (1963). *Magnetism* (Academic Press, New York).
- Benelli, C., Gatteschi, D. (2015). *Introduction to Molecular Magnetism: From Transition Metals to Lanthanides* (Wiley-VCH, Weinheim).
- Blundell, S. (2001). *Magnetism in Condensed Matter* (Oxford University Press, Oxford).
- Canadell, E., Doublet, M.-L., Jung, C. (2012). *Orbital Approach to the Electronic Structure of Solids* (Oxford University Press, Oxford).
- Carlin, R. L. (1986). *Magnetochemistry* (Springer-Verlag, Berlin, Heidelberg, New York, Tokyo).
- Coey, J. M. D. (2010). *Magnetism and Magnetic Materials* (Cambridge University Press, Cambridge).
- Coronado, E., Day, P. (2004). *Magnetic molecular conductors*, *Chem. Rev.*, 104, pp. 5419–5448.
- Cotton, F. A. (1990). *Chemical Applications of Group Theory, Chapter 7* (Wiley, New York).
- Fourmigué, M., Ouahab, L. (eds.) (2009). *Conducting and Magnetic Organometallic Molecular Materials* (Springer, Berlin).
- Gatteschi, D., Sessoli, R., Villain, J. (2006). *Molecular Nanomagnets* (Oxford University Press, Oxford).
- Goodenough, J. B. (1966). *Magnetism and the Chemical Bond* (Interscience Publisher, New York).

Halcrow, M. A. (ed.) (2013). *Spin-Crossover Materials: Properties and Applications* (Wiley-WCH, Hoboken). Hung, L. S., Chen, C. H. (2002). Recent progress of molecular organic electroluminescent materials and devices, *Mater. Sci. Eng. R*, 39, pp.143–222.

Kahn, O. (1993). *Molecular Magnetism* (Wiley-VCH, New York).

Kalyanasundaram, K., Grätzel, M. (1998). Applications of functionalized transition metal complexes in photonic and optoelectronic devices, *Coord. Chem. Rev.*, 77, pp. 347–414.

Launay, J.-P., Verdager, M. (2014). *Electrons in Molecules: From Basic Principles to Molecular Electronics* (Oxford University Press, Oxford).

Marder, S. R., Sohn, J. E., Stucky, G. D. (eds.) (1991). *Materials for Nonlinear Optics: Chemical Perspectives* (American Chemical Society, Washington).

Nielsen, M., Chuang, I. (2004). *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge).

Peierls, R. E. (1955). *Quantum Theory of Solids* (Oxford University Press, Oxford).

Pilkington, M., Decurtins, S. (2002). Oxalate-based 2D and 3D magnets, in *Magnetism: Molecules to Materials II: Molecule-Based Materials*, Miller, J. S., Drillon, M., eds. (Wiley-VCH, Weinheim).

Robertson, N., Yee, G. T. (2010). Molecular magnetic materials, in *Molecular Materials*, Bruce, D. W., O'Hare, D., Walton, R. I., eds. (Wiley-WCH, Weinheim).

Shultz, D. A. (2002). Valence tautomerism in dioxolene complexes of cobalt, in *Magnetism: Molecules to Materials II: Molecule-Based Materials*, Miller, J. S., Drillon, M., eds. (Wiley-VCH, Weinheim).

Tanner, B. (1995). *Introduction to the Physics of Electrons in Solids* (Cambridge University Press, Cambridge).

West, A. R. (1999). *Basic Solid State Chemistry*, 2nd ed. (John Wiley & Sons, Chichester,).

Winpenny, R. E. P. (ed.) (2012). *Molecular Cluster Magnets* (World Scientific Publishing, Singapore).

Winpenny, R. E. P., McInnes, E. J. L. (2010). Molecular nanomagnets, in *Molecular Materials*, Bruce, D. W., O'Hare, D., Walton, R. I., eds. (Wiley-VCH, Weinheim).

# Chemistry of nano- and biomaterials

## COURSE OUTLINE

### 1. GENERAL

SCHOOL	NATURAL SCIENCES		
ACADEMIC UNIT/PARTICIPATING UNITS	MATERIALS SCIENCE		
PARTICIPATING INSTITUTIONS			
POSTGRADUATE PROGRAMME: TITLE OF POSTGRADUATE PROGRAMME	Materials Science		
LEVEL OF STUDIES	Postgraduate		
COURSE CODE	<b>EY-B5.1</b>	SEMESTER	2 <sup>nd</sup>
COURSE TITLE	Chemistry of nano- and biomaterials		
INDEPENDENT TEACHING ACTIVITIES	WEEKLY TEACHING HOURS	CREDITS	
	3	6	
COURSE TYPE	Scientific area		
PREREQUISITE COURSES:	NO		
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek or English if it is required		
IS THE COURSE OFFERED TO ERASMUS STUDENTS	YES (as reading course)		
COURSE WEBSITE (URL)	<a href="https://www.matersci.upatras.gr/el/studies/postgraduate/epistimi-ton-ylikon/msccourses">https://www.matersci.upatras.gr/el/studies/postgraduate/epistimi-ton-ylikon/msccourses</a>		

### 2. LEARNING OUTCOMES

Learning outcomes
At the end of this course the student will have a deep knowledge on the modern chemical treatments that are involved in the preparation and the chemical modification of nanoscale materials. The student will be able to select and propose and study such chemical treatment for the preparation of new nanomaterials and to study their role in size, shape, structure and chemical composition.
<i>The course belongs to Levels 7 of the European Qualifications Framework for Lifelong Learning.</i>
General Competences
<i>Seeking, analyzing and composing data and information by employing necessary technologies. Autonomous working Team working Working in a multi discipline environment Protecting natural environment.</i>

### 3. SYLLABUS

Introduction in nanostructured materials. Metal nanoparticles (gold, silver, iron oxides), carbon nanostructures (nanotubes, graphene, nanodots), 2D Van der Waals and non van der Waals materials. Method of preparations wet chemistry – reduction of metal cations – oxidation and reduction of graphene. Liquid phase exfoliation with sonication. Surface treatment of nanomaterials. Hydrothermal treatment. Aerogels, hydrogels and doping with nanoparticles.

### 4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY.	Face to face (presentation in the classroom)		
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY	Lectures using slides for overhead projector or power point presentation as well as classic class board. Study of selected scientific articles from the students.		
TEACHING METHODS	<b>Activity</b>	<b>Semester workload</b>	
	Lectures	50	
	Study-Search of Bibliography	50	
	Discussion-Bibliography analysis	50	
	Course total	<b>150</b>	
STUDENT PERFORMANCE EVALUATION	<p>Combination of oral examination and a presentation of a selected project.</p> <p style="text-align: center;"><b>General criteria for the assessment of students</b></p> <p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course.</p>		

### 5. RECOMMENDED BIBLIOGRAPHY

**- Suggested bibliography:**

**Broad Family of Carbon Nanoallotropes: Classification, Chemistry, and Applications of Fullerenes, Carbon Dots, Nanotubes, Graphene, Nanodiamonds, and Combined Superstructures.** V Georgakilas, Jason A. Perman, Jiri Tucek, Radek Zboril, Chem. Rev. 2015, 115, 4744–4822.

**Recent Advances in the Liquid-Phase Syntheses of Inorganic Nanoparticles.** Brian L. Cushing, Vladimir L. Kolesnichenko, Charles J. O'Connor, Chemical Reviews, 2004, 104.

**Gold Nanoparticles: Assembly, Supramolecular Chemistry, Quantum-Size-Related Properties, and Applications toward Biology, Catalysis, and Nanotechnology.** Marie-Christine Daniel and Didier Astruc, Chem. Rev. 2004, 104, 293-346.

**Nanoscience, Nanotechnology, and Chemistry.** George M. Whitesides, small 2005, 1, 172 –179.

**Soft Nanotechnology with Soft Nanoparticles.** Satish Nayak, L. Andrew Lyon. Angew. Chem. Int. Ed. 2005, 44, 7686 – 7708

**- Related academic journals:**  
*Chemical Reviews, Journal of Materials Chemistry, ACS Applied materials & Interfaces, ACS Applied Nanomaterials, Nanomaterials, Green Chemistry*

# Advanced Composite and Hybrid Materials

## COURSE OUTLINE

### 1. GENERAL

SCHOOL	NATURAL SCIENCES		
ACADEMIC UNIT/PARTICIPATING UNITS	MATERIALS SCIENCE		
PARTICIPATING INSTITUTIONS			
POSTGRADUATE PROGRAMME: TITLE OF POSTGRADUATE PROGRAMME	Materials Science		
LEVEL OF STUDIES	Postgraduate		
COURSE CODE	EY-B6.1	SEMESTER	2 <sup>nd</sup>
COURSE TITLE	Advanced Composite and Hybrid Materials		
INDEPENDENT TEACHING ACTIVITIES	WEEKLY TEACHING HOURS	CREDITS	
	2	6	
COURSE TYPE	Specialised general knowledge		
PREREQUISITE COURSES:	NO		
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek or English if it is required		
IS THE COURSE OFFERED TO ERASMUS STUDENTS	YES		
COURSE WEBSITE (URL)	<a href="https://www.matersci.upatras.gr/el/studies/postgraduate/epistimi-ton-ylikon/msccourses">https://www.matersci.upatras.gr/el/studies/postgraduate/epistimi-ton-ylikon/msccourses</a>		

### 2. LEARNING OUTCOMES

Learning outcomes
<p>With the successful completion of the course students will be able:</p> <ol style="list-style-type: none"> <li>1. Identify and classify the advanced composite and hybrid materials.</li> <li>2. To describe the basic methods of fabricating composite and nanocomposite materials.</li> <li>3. Understand the mechanical behaviour and response of composite and hybrid materials, their dielectric properties and conductivity, their magnetic properties, the role of the interface and to quantify the influence of the reinforcing phase.</li> <li>4. Understand the concept and the operation of multifunctional nanocomposite/hybrid materials of polymer matrix.</li> </ol>
General Competences

- Search for, analysis and synthesis of data and information, with the use of the necessary technology - Adapting to new situations
- Working independently
- Team work
- Working in an international environment
- Working in an interdisciplinary environment
- Production of new research ideas
- Project planning and management
- Respect for the natural environment
- Criticism and self-criticism
- Production of free, creative and inductive thinking

### 3. SYLLABUS

Technological importance of nanocomposites and hybrid materials. Types and categories of composite materials. Nanocomposites. Methods of fabrication. Properties and applications. Mechanical behaviour and response. Dielectric response and conductivity. Magnetic properties. Interface and its importance. Polymer matrix multifunctional nanocomposite/hybrid materials.

### 4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY	Face-to-face	
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY	Teaching of the course is carried out via weekly lectures with slides via a video projector, where the theory is thoroughly analysed and are presented examples from the scientific literature. Students are motivated to seek for relative papers and to conduct a project which will present in the class.	
TEACHING METHODS	<i>Activity</i>	<i>Semester workload</i>
	Lectures	39
	Studying-Literature research	60
	Writing bibliographic essays reports/project presentation	51
	Course total	150
STUDENT PERFORMANCE EVALUATION	<p>Students are evaluated by writing and presenting a relative project.</p> <p style="text-align: center;"><b>General criteria for the assessment of students</b></p> <p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course.</p>	

### 5. RECOMMENDED BIBLIOGRAPHY

- *Suggested bibliography:*

Song, K.; Guo, J.Z.; Liu, C. *Polymer-Based Multifunctional Nanocomposites and Their Applications*; Elsevier: Amsterdam, 2019; ISBN 9780128150672.

Friedrich, K. Routes for achieving multifunctionality in reinforced polymers and composite structures. In *Multifunctionality of Polymer Composites*; Friedrich, K., Breuer, U., Eds.; Elsevier, 2015; pp. 3–41 ISBN 978-0-32326434-1.

Psarras, G.C. Ceramic/Polymer Nanodielectrics: Towards A Multifunctional Or Smart Performance. In *Proceedings of the ECCM18 - 18th European Conference on Composite Materials*; Athens, Greece, 2018; pp. 24–28. Dang, Z.-M.; Wang, L.; Yin, Y.; Zhang, Q.; Lei, Q.-Q. Giant Dielectric Permittivities in Functionalized CarbonNanotube/ Electroactive-Polymer Nanocomposites. *Adv. Mater.* 2007, 19, 852–857.

- *Related academic journals:*

Advanced Functional Materials, Advanced Materials, Express Polymer Letters, Polymer, Composites part A, Composite Science and Technology.

# Special Topics in Materials Science

## COURSE OUTLINE

### 1. GENERAL

SCHOOL	NATURAL SCIENCES		
ACADEMIC UNIT/PARTICIPATING UNITS	MATERIALS SCIENCE		
PARTICIPATING INSTITUTIONS			
POSTGRADUATE PROGRAMME: TITLE OF POSTGRADUATE PROGRAMME	Materials Science		
LEVEL OF STUDIES	Postgraduate		
COURSE CODE	EY-B7.1	SEMESTER	2 <sup>nd</sup>
COURSE TITLE	Special Topics in Materials Science		
INDEPENDENT TEACHING ACTIVITIES		WEEKLY TEACHING HOURS	CREDITS
		2	6
COURSE TYPE	Specialised general knowledge		
PREREQUISITE COURSES:	NO		
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek or English if it is required		
IS THE COURSE OFFERED TO ERASMUS STUDENTS	YES		
COURSE WEBSITE (URL)	<a href="https://www.matersci.upatras.gr/el/studies/postgraduate/epistimionylikon/msc-courses">https://www.matersci.upatras.gr/el/studies/postgraduate/epistimionylikon/msc-courses</a> .		

### 2. LEARNING OUTCOMES

Learning outcomes
The specific course has not been offered to students as yet. Its structure will be a series of seminars relative to new, modern experimental techniques in the field of materials science, which cannot be developed in Greece because of their cost. Instructors will be visiting professors. With the successful completion of the course students will be familiar with these experimental techniques
General Competences
<ul style="list-style-type: none"> <li>- Search for, analysis and synthesis of data and information, with the use of the necessary technology - Adapting to new situations</li> <li>- Working independently</li> <li>- Team work</li> <li>- Working in an international environment</li> <li>- Working in an interdisciplinary environment</li> <li>- Production of new research ideas</li> <li>- Project planning and management</li> <li>- Respect for the natural environment</li> <li>- Criticism and self-criticism</li> <li>- Production of free, creative and inductive thinking</li> </ul>

### 3. SYLLABUS

The course has not been offered to students as yet. It will be composed by weekly seminars. Students will be motivated to search for relative literature and to make a relative project.

#### 4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY.	Face-to-face		
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY	Teaching of the course is carried out via weekly lectures with slides via a video projector, where the theory is thoroughly analysed and are presented examples from the scientific literature. Students are motivated to seek for relative papers and to conduct a project which will present in the class.		
TEACHING METHODS	<i>Activity</i>	<i>Semester workload</i>	
	Lectures	39	
	Studying-Literature research	60	
	Writing bibliographic essays reports/project presentation	51	
	<b>Course total</b>	<i>150</i>	
STUDENT PERFORMANCE EVALUATION	<p>Students are evaluated by writing and presenting a relative project.</p> <p style="text-align: center;"><b>General criteria for the assessment of students</b></p> <p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course.</p>		

#### 5. RECOMMENDED BIBLIOGRAPHY

- *Suggested bibliography:*

Because of the nature of the course, specific bibliography cannot be recommended. - *Related academic journals:*

## Direction B'

### Quantum Phenomena in Materials. Ab initio Modelling and Simulations

#### COURSE OUTLINE

##### 1. GENERAL

SCHOOL	Naturals Sciences		
ACADEMIC UNIT/PARTICIPATING UNITS	Materials Science		
PARTICIPATING INSTITUTIONS			
POSTGRADUATE PROGRAMME: TITLE OF POSTGRADUATE PROGRAMME	Materials Science		
LEVEL OF STUDIES	Postgraduate		
COURSE CODE	<b>EY-B1.2</b>	SEMESTER	2 <sup>nd</sup>
COURSE TITLE	Quantum Phenomena in Materials. Ab initio Modeling and Simulations		
INDEPENDENT TEACHING ACTIVITIES	WEEKLY TEACHING HOURS	CREDITS	
	3	7	
COURSE TYPE	Specialized general knowledge		
PREREQUISITE COURSES:	NO		
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek (English if needed)		
IS THE COURSE OFFERED TO ERASMUS STUDENTS	Yes		
COURSE WEBSITE (URL)	<a href="https://www.matersci.upatras.gr/el/studies/postgraduate/epistimi-ton-ylikon/msccourses">https://www.matersci.upatras.gr/el/studies/postgraduate/epistimi-ton-ylikon/msccourses</a>		

##### 2. LEARNING OUTCOMES

Learning outcomes
At the end of the course the student will have come into contact with the basic methods of electronic structure as they are applied to computational studies of molecules, nanostructures, surfaces and solids and will have familiarized himself with the use of popular computational tools. He will be able to recognize the advantages and disadvantages of various methods/approaches and programs for common types of calculations and will be able to select best practices for simulating a multitude of electronic, optical and structural properties of realistic systems from the field of materials science. Finally, he will be able to properly process, visualize and present the results of calculations. The course according to the European Qualifications Framework for Lifelong Learning is level 7 as a second cycle course.
General Competences
Search for, analysis and synthesis of data and information, with the use of the necessary technology Working independently Team work Production of new research ideas

Production of free, creative and inductive thinking

### 3. Syllabus

Introduction to Density Functional Theory. Solving the electronic problem. Categorization of methods from first principles. The problem of electronic structure in materials. Quantum Many-Body Theory. Hartree & Hartree-Fock methods. Density Functional Theory (DFT). Exchange & correlation in DFT. Solution of the one-electron problem and self-consistency: Hartree-Fock & Kohn-Sham equations. Atomic Pseudopotentials. Bases for the development of real wave functions. Electronic structure methods: KKR, all-electron, pseudopotential plane waves, atom-centered basis sets, Gaussian and related methods, real-space methods. Alternative approaches to the electronic problem: Tight binding, semi-empirical, hybrid QM-MM etc. Competition, self-consistency and convergence to a solution. Quantum molecular dynamics from first principles

### 4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY	Face-to-face		
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY	The teaching of the course takes place both in a classroom and in the computer center where each student has access to a personal computer and to the use of software, as a rule open source.		
TEACHING METHODS	<i>Activity</i>	<i>Semester workload</i>	
	Lectures in a classroom/computer center	39	
	Elaboration, Writing and Presentation of Assignments	55	
	Literature study & analysis	78	
	Final exam	3	
	Course total	175	
STUDENT PERFORMANCE EVALUATION	<p>Assignments and presentations during the semester. Written or oral exam at the end of the semester. The final grade results from the laboratory reports, and from an examination during the public presentation of the laboratory exercises concerning computational modeling and problem solving as well as from the final written or oral examination.</p> <p style="text-align: center;"><b>General criteria for the assessment of students</b></p> <p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course.</p>		

### 5. RECOMMENDED BIBLIOGRAPHY

- Wolfram Koch, Max C. Holthausen, A Chemist's Guide to Density Functional Theory, Wiley-VCH 2001
- Frank Jensen, Introduction to Computational Chemistry, Wiley 2007.
- J. B. Foresman and A. Frisch, 3rd ed., Gaussian, Inc.: Wallingford, CT, 2015.

- Walter Harrison, *Electronic Structure and the Properties of Solids*, Dover, 1989.
- K. Ohno, K. Esfarjani, Y. Kawazoe, *Computational Materials Science: From Ab Initio to Monte Carlo Methods*, Springer, 1999.
- Eftimos Kaxiras, *Atomic and Electronic Structure of Solids*, Cambridge University Press, 2003.
- Richard Martin, *Electronic Structure: Basic Theory and Practical Methods*, Cambridge University Press, 2004.
- Jorge Kohanoff, *Electronic Structure Calculations for Solids and Molecules*, Cambridge University Press, 2006.

# Multi Scale Modeling of Materials and Simulation Techniques. From nano to macro

## COURSE OUTLINE

### 1. GENERAL

SCHOOL	NATURAL SCIENCES		
ACADEMIC UNIT	DEPARTMENT OF MATERIALS SCIENCE		
PARTICIPATING INSTITUTIONS			
POSTGRADUATE PROGRAMME: TITLE OF POSTGRADUATE PROGRAMME	MATERIALS SCIENCE		
LEVEL OF STUDIES	7 <sup>th</sup> (Master Degree)		
COURSE CODE	EY_B2.2	SEMESTER	2 <sup>nd</sup>
COURSE TITLE	Multi Scale Modelling of Materials and Simulation Techniques. From nano to macro.		
<b>INDEPENDENT TEACHING ACTIVITIES</b>		<b>WEEKLY TEACHING HOURS</b>	<b>CREDITS</b>
		3	7
COURSE TYPE	special background		
PREREQUISITE COURSES:	NONE		
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek (English if needed)		
IS THE COURSE OFFERED TO ERASMUS STUDENTS	yes		
COURSE WEBSITE (URL)	<a href="https://www.matersci.upatras.gr/images/joomlart/university/docs/PMS/Msc_Materials_Science_Sintomos_Odigos.pdf">https://www.matersci.upatras.gr/images/joomlart/university/docs/PMS/Msc_Materials_Science_Sintomos_Odigos.pdf</a>		

### 2. LEARNING OUTCOMES

<b>Learning outcomes</b>
Classical models for describing intermolecular interactions between complex molecular structures are introduced. Monte Carlo and Molecular Dynamics molecular simulation techniques are developed in detail. Molecular simulations in various statistical collections: microcanonical, isochronous, isobaric and thermostating and barostating methods are discussed. The finite element method in modelling macroscopic properties of materials of technological interest. The course, according to the European Qualifications Framework for Lifelong Learning, is at level 7 as a postgraduate program.
<b>General Competences</b>
Search for, analysis and synthesis of data and information, Working independently, Team work, Production of new research ideas, Production of free, creative and inductive thinking

### 3. SYLLABUS

Review of probability and statistical mechanical concepts. Intermolecular potential, atomistic and coarse-grained models. Electrostatic interactions. Classical force fields. Polyatomic molecules and intra-molecular potentials. Simulations with periodic conditions and the minimum image convention. The method of classical molecular dynamics simulations. Thermostats, Barostats and simulations of systems in the NVE, NVT and NpT ensembles.

Basic principles of the Monte Carlo Method. Analysing the results of the molecular simulations, structure, order parameters and phase transformations. In addition, the finite difference method is presented in one, two and three dimensions. There will be an extensive presentation of the accuracy of the method as well as the absorbing boundary conditions. Its applications in electromagnetic, elastic and acoustic wave propagation will be presented. The finite element method is presented and compared to the finite difference method. Application of the method to the propagation of electromagnetic, elastic and acoustic waves.

#### 4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY	Face-to-face		
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY	Teaching includes use of ICT as well as whiteboard for in depth presentation of theory and problem solving		
TEACHING METHODS	<b>Activity</b>	<b>Semester workload</b>	
	lectures	39	
	Home work	75	
	Study and analysis of bibliography	61	
	Course total	<b>175</b>	
STUDENT PERFORMANCE EVALUATION	<p>Problem solving during written final exam.</p> <p style="text-align: center;"><b>General criteria for the assessment of students</b></p> <p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course.</p>		

#### 5. RECOMMENDED BIBLIOGRAPHY

*Frenkel, D., Smit, B. Understanding Molecular Simulation: From Algorithms to Applications. Academic Press, 1996.*

*Allen, M.P., Tildesley, D.J. Computer Simulation of Liquids. Oxford University Press, 2017.*

*LeSar, R. Introduction to Computational Materials Science: Fundamentals to Applications. Cambridge University Press, 2013.*

*Rumpf, R.C. Electromagnetic and Photonic Simulation for the Beginner: Finite-Difference Frequency-Domain in MATLAB®. Artech House, 2022.*

# Master Thesis I

## COURSE OUTLINE

### 1. GENERAL

SCHOOL	NATURAL SCIENCES		
ACADEMIC UNIT/PARTICIPATING UNITS	MATERIALS SCIENCE		
PARTICIPATING INSTITUTIONS			
POSTGRADUATE PROGRAMME: TITLE OF POSTGRADUATE PROGRAMME	Materials Science		
LEVEL OF STUDIES	Postgraduate		
COURSE CODE	EY-MT1.2	SEMESTER	2 <sup>nd</sup>
COURSE TITLE	Master Thesis I		
INDEPENDENT TEACHING ACTIVITIES	WEEKLY TEACHING HOURS	CREDITS	
	-	10	
COURSE TYPE	Specialised general knowledge		
PREREQUISITE COURSES:	NO		
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek or English if it is required		
IS THE COURSE OFFERED TO ERASMUS STUDENTS	YES		
COURSE WEBSITE (URL)	-		

### 2. LEARNING OUTCOMES

Learning outcomes
Conducting Master Thesis I. In the first part of the Thesis is conducted bibliographic survey of the subject. The subject of the Thesis is determined in collaboration with the Supervising Professor.
General Competences
<ul style="list-style-type: none"> <li>- Search for, analysis and synthesis of data and information, with the use of the necessary technology - Adapting to new situations</li> <li>- Working independently</li> <li>- Team work</li> <li>- Working in an international environment</li> <li>- Working in an interdisciplinary environment</li> <li>- Production of new research ideas</li> <li>- Project planning and management</li> <li>- Respect for the natural environment</li> <li>- Criticism and self-criticism</li> <li>- Production of free, creative and inductive thinking</li> </ul>

### 3. SYLLABUS

Bibliographic survey of the Thesis's subject.

#### 4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY.	Face-to-face	
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY	Using electronic (web) tools for literature search.	
TEACHING METHODS	<i>Activity</i>	<i>Semester workload</i>
	Studying-Literature research	100
	Writing bibliographic essays reports/project presentation	150
	<b>Course total</b>	<b>250</b>
STUDENT PERFORMANCE EVALUATION	<p>Students are evaluated via the conducted bibliographic survey and the writing of the theoretical part of their Thesis.</p> <p style="text-align: center;"><b>General criteria for the assessment of students</b></p> <p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course.</p>	

#### 5. RECOMMENDED BIBLIOGRAPHY

- *Suggested bibliography:*

Because of the nature of the course, specific bibliography cannot be recommended. - *Related academic journals:*

# Molecular Simulations of Soft Materials and Biomolecular Systems

## COURSE OUTLINE

### 1. GENERAL

SCHOOL	NATURAL SCIENCES		
ACADEMIC UNIT	DEPARTMENT OF MATERIALS SCIENCE		
PARTICIPATING INSTITUTIONS			
POSTGRADUATE PROGRAMME: TITLE OF POSTGRADUATE PROGRAMME	MATERIALS SCIENCE		
LEVEL OF STUDIES	7 <sup>th</sup> (Master Degree)		
COURSE CODE	EY_B3.2	SEMESTER	2 <sup>nd</sup>
COURSE TITLE	Molecular Simulations of Soft Materials and Biomolecular Systems.		
<b>INDEPENDENT TEACHING ACTIVITIES</b>	<b>WEEKLY TEACHING HOURS</b>	<b>CREDITS</b>	
	3	6	
COURSE TYPE	special background		
PREREQUISITE COURSES:	None		
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek/English if needed		
IS THE COURSE OFFERED TO ERASMUS STUDENTS	yes		
COURSE WEBSITE (URL)	<a href="https://www.matersci.upatras.gr/images/joomlart/university/docs/PMS/Msc_Materials_Science_Sintomos_Odigos.pdf">https://www.matersci.upatras.gr/images/joomlart/university/docs/PMS/Msc_Materials_Science_Sintomos_Odigos.pdf</a>		

### 2. LEARNING OUTCOMES

<b>Learning outcomes</b>
<p>Models of macromolecules, linear, branched, dendritic macromolecules. Conformations, intramolecular interactions, and nanomechanics. Electrostatic interactions, the role of the solvent in molecular properties. Specific interactions (hydrogen bonds, <math>\pi</math>-<math>\pi</math>, etc.) and their role in molecular self-assembly and self-organization in molecular and biomolecular systems. Molecular field theories and functional density theories. Simulations of molecular dynamics with open-source software.</p> <p>The course, according to the European Qualifications Framework for Lifelong Learning, is at level 7 as a postgraduate program.</p>
<b>General Competences</b>
Search for, analysis and synthesis of data and information, Working independently, Team work, Production of new research ideas, Production of free, creative and inductive thinking

### 3. SYLLABUS

Ideal macromolecular chains, freely-jointed chains and the worm-like chain model. Excluded volume interactions. Elastic properties and mechanical response of macromolecules. Electrostatic interactions, screening. Weak interactions and macromolecular self-organization. Helix-coil transition in biomolecules. Various organization levels in biomacromolecules. Emergence of larger scale supermolecular biological structures. Molecular dynamics simulations and coarse-grained models. The Peyrard-Bisho-Dauxois model for the thermal openings and the denaturation of DNA double helix.

#### 4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY	Face-to-face		
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY	Teaching includes use of ICT as well as whiteboard for in depth presentation of theory and problem solving		
TEACHING METHODS	<b>Activity</b>	<b>Semester workload</b>	
	lectures	39	
	Home work	60	
	Study and analysis of bibliography	51	
	Course total	<b>150</b>	
STUDENT PERFORMANCE EVALUATION	<p>Problem solving during written final exam</p> <p style="text-align: center;"><b>General criteria for the assessment of students</b></p> <p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course.</p>		

#### 5. RECOMMENDED BIBLIOGRAPHY

- 19) *Molecular driving forces: Statistical Thermodynamics in Biology, Chemistry, Physics, and Nanoscience*, 2<sup>nd</sup> Ed., Ken A. Dill and Sabrina Bromberg, Taylor & Francis (2011)
- 20) *Concepts in Thermal Physics*, S. J. Blundell and K. M. Blundell, Oxford University Press (2010)
- 21) *Atkins' Physical Chemistry*, P. Atkins and J. De Paula, 8<sup>th</sup> Ed. Oxford University Press (2006)
- 22) *Fundamentals and Applications of Controlled Release Drug Delivery*, Eds. Siepmann, Siegel, and Rathbone, Springer (2012)

# Mesoscopic Simulations of Materials and Functional Devices (Thermal, Mechanical, Electric, Photonic and Phononic Properties)

## COURSE OUTLINE

### 1. GENERAL

SCHOOL	NATURAL SCIENCES		
ACADEMIC UNIT	DEPARTMENT OF MATERIALS SCIENCE		
PARTICIPATING INSTITUTIONS			
POSTGRADUATE PROGRAMME: TITLE OF POSTGRADUATE PROGRAMME	MATERIALS SCIENCE		
LEVEL OF STUDIES	7 <sup>th</sup> (Master Degree)		
COURSE CODE	EY_B4.2	SEMESTER	2 <sup>nd</sup>
COURSE TITLE	Mesoscopic Simulations of Materials and Functional Devices (Thermal, Mechanical, Electric, Photonic and Phononic Properties)		
<b>INDEPENDENT TEACHING ACTIVITIES</b>		<b>WEEKLY TEACHING HOURS</b>	<b>CREDITS</b>
		3	10
COURSE TYPE	special background		
PREREQUISITE COURSES:	None		
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek (English if needed)		
IS THE COURSE OFFERED TO ERASMUS STUDENTS	yes		
COURSE WEBSITE (URL)	<a href="https://www.matersci.upatras.gr/images/joomlart/university/docs/PMS/Msc_Materials_Science_Sintomos_Odigos.pdf">https://www.matersci.upatras.gr/images/joomlart/university/docs/PMS/Msc_Materials_Science_Sintomos_Odigos.pdf</a>		

### 2. LEARNING OUTCOMES

Learning outcomes
<p>Simulation methods for Materials and Devices with dimensions ranging from a few hundred nanometers to several micrometers will be presented. The general characteristics, as well as the disadvantages and advantages of these methods, will be developed. Applications of various methods in different materials and devices will be examined and compared with experimentation. Indicatively, some of the methods to be presented include: Waveguide Level Development, Finite Differences, Finite Elements. Selected studies using available computational packages will be discussed. The course, according to the European Qualifications Framework for Lifelong Learning, is at level 7 as a postgraduate program.</p>
General Competences
<p>Search for, analysis and synthesis of data and information, Working independently, Team work, Production of new research ideas, Production of free, creative and inductive thinking</p>

### 3. SYLLABUS

<p>The topics discussed in the courses include: Molecular Dynamics: MD, ab initio MD, time-stepping algorithms, classical</p>
---

MD, Born-Oppenheimer MD, thermostats. Basic DFT: Born-Oppenheimer and Hartree Fock approaches, ThomasFermi, Hohenberg-Kohn, LDA, GGA, DFT practices, geometry optimization methods, pseudodynamics. Transfer matrix methods and FDTD are presented and applied to materials, including quantum nanostructures, as well as photonic materials and structures. We present computations with time-dependent density functional theory and calculations with plane-wave density functional theory using open-source computational packages.

#### 4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY	Face-to-face		
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY	Teaching includes use of ICT as well as whiteboard for in depth presentation of theory and problem solving		
TEACHING METHODS	<b>Activity</b>	<b>Semester workload</b>	
	lectures	39	
	Course assignments	30	
	Study and analysis of bibliography	31	
	Semester project	40	
	Course total	<b>150</b>	
STUDENT PERFORMANCE EVALUATION	<p>Evaluation with semester project and assignments during the course.</p> <p style="text-align: center;"><b>General criteria for the assessment of students</b></p> <p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course.</p>		

#### 5. RECOMMENDED BIBLIOGRAPHY

*Computational Materials Science: Fundamentals to Applications*, Richard Lesar, Cambridge University Press (2013)  
*Computational Nanoscience*, Kalman Varga and Joseph A. Driscoll, Cambridge University Press (2011)  
*Computer Simulations of Liquids, 2<sup>nd</sup> Ed.*, Michael P. Allen and Dominic J. Tildesley, Oxford University Press (2017)  
*Numerical Electromagnetics: The FDTD method*, Umran S. Inan and Robert A. Marshall, Cambridge University Press (2011)  
*Electronic Structure: Basic Theory and Practical Methods, 2<sup>nd</sup> Ed.*, Richard M. Martin, Cambridge University Press (2020)

# Theory and Simulations of Electronic, Magnetic and Optical properties of Nanomaterials

## COURSE OUTLINE

### 1. GENERAL

SCHOOL	NATURAL SCIENCES		
ACADEMIC UNIT	DEPARTMENT OF MATERIALS SCIENCE		
PARTICIPATING INSTITUTIONS			
POSTGRADUATE PROGRAMME: TITLE OF POSTGRADUATE PROGRAMME	MATERIALS SCIENCE		
LEVEL OF STUDIES	7 <sup>th</sup> (Master Degree)		
COURSE CODE	EY_B5.2	SEMESTER	2 <sup>nd</sup>
COURSE TITLE	Theory and Simulations of Electronic, Magnetic and Optical properties of Nanomaterials		
<b>INDEPENDENT TEACHING ACTIVITIES</b>		<b>WEEKLY TEACHING HOURS</b>	<b>CREDITS</b>
		3	6
COURSE TYPE	special background		
PREREQUISITE COURSES:	None		
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek/English if needed		
IS THE COURSE OFFERED TO ERASMUS STUDENTS	yes		
COURSE WEBSITE (URL)	<a href="https://www.matersci.upatras.gr/images/joomlart/university/docs/PMS/Msc_Materials_Science_Sintomos_Odigos.pdf">https://www.matersci.upatras.gr/images/joomlart/university/docs/PMS/Msc_Materials_Science_Sintomos_Odigos.pdf</a>		

### 2. LEARNING OUTCOMES

Learning outcomes
<p>Effect of size on the electronic, magnetic, and optical properties of materials. The theoretical background upon which specific electronic structure software packages are based. Familiarization with specific software and its use for determining the electronic, magnetic, and optical properties of nanomaterials.</p> <p>The course, according to the European Qualifications Framework for Lifelong Learning, is at level 7 as a postgraduate program.</p>
General Competences
Search for, analysis and synthesis of data and information, Working independently, Team work, Production of new research ideas, Production of free, creative and inductive thinking

### 3. SYLLABUS

In the theory part of the course the following topics are discussed: Review of semiconductor physics, basic properties of low-dimensional structures, semiconductor quantum nanostructures, multiple quantum wells, and superlattices, electric field transport in nanostructures, optical and electrooptical processes in low-dimensional quantum structures and applications, such as electronic, photonic and optoelectronic devices based on nanostructures. Computational packages and open-source codes will be used for simulating the above-mentioned processes in the computational laboratory part of the course.

#### 4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY	Face-to-face	
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY	Teaching includes use of ICT as well as whiteboard for in depth presentation of theory and problem solving	
TEACHING METHODS	<b>Activity</b>	<b>Semester workload</b>
	lectures	21
	Computational lab assignments	18
	assignments	60
	Study and analysis of bibliography	51
	Course total	<b>150</b>
STUDENT PERFORMANCE EVALUATION	<p>Problem solving during written final exam and evaluation of assignments during the course</p> <p style="text-align: center;"><b>General criteria for the assessment of students</b></p> <p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course.</p>	

#### 5. RECOMMENDED BIBLIOGRAPHY

*Introduction to Nanophotonics, 2<sup>nd</sup> Ed.*, Sergey V. Gaponenko, Cambridge University Press (2010).  
*Quantum Mechanics: An Introduction for Device Physicists and Electrical Engineers, 2<sup>nd</sup> Ed.*, David K. Ferry, IoP Publishing (2001)  
*Optoelectronics*, Emmanuel Rosencher and Borge Vinter, Cambridge University Press (2004)  
*Numerical Electromagnetics: The FDTD method*, Umran S. Inan and Robert A. Marshall, Cambridge University Press (2011)  
*Electromagnetic Simulation Using the FDTD method with Python, 3<sup>rd</sup> Ed.*, Jennifer E. Houle and Dennis M. Sullivan, IEEE Press Wiley (2020)  
*Nanotechnology for Microelectronics and Photonics, 2<sup>nd</sup> Ed.*, Raul J. Martin-Palma and Jose M. Martinez-Duarte, Elsevier (2017)

# Special Topics in Computational Materials Science

## COURSE OUTLINE

### 1. GENERAL

SCHOOL	NATURAL SCIENCES		
ACADEMIC UNIT	DEPARTMENT OF MATERIALS SCIENCE		
PARTICIPATING INSTITUTIONS			
POSTGRADUATE PROGRAMME: TITLE OF POSTGRADUATE PROGRAMME	MATERIALS SCIENCE		
LEVEL OF STUDIES	7 <sup>th</sup> (Master Degree)		
COURSE CODE	EY_B6.2	SEMESTER	2 <sup>nd</sup>
COURSE TITLE	Special Topics in Computational Materials Science		
<b>INDEPENDENT TEACHING ACTIVITIES</b>	<b>WEEKLY TEACHING HOURS</b>	<b>CREDITS</b>	
	3	6	
COURSE TYPE	Specialised general knowledge		
PREREQUISITE COURSES:	None		
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek/English if needed		
IS THE COURSE OFFERED TO ERASMUS STUDENTS	yes		
COURSE WEBSITE (URL)	<a href="https://www.matersci.upatras.gr/images/joomlart/university/docs/PMS/Msc_Materials_Science_Sintomos_Odigos.pdf">https://www.matersci.upatras.gr/images/joomlart/university/docs/PMS/Msc_Materials_Science_Sintomos_Odigos.pdf</a>		

### 2. LEARNING OUTCOMES

<b>Learning outcomes</b>
Advanced specialized seminar lectures on new and emerging techniques and methodologies on computational materials science. The course, according to the European Qualifications Framework for Lifelong Learning, is at level 7 as a postgraduate program.
<b>General Competences</b>
Search for, analysis and synthesis of data and information, Working independently, Team work, Production of new research ideas, Production of free, creative and inductive thinking.

### 3. SYLLABUS

Seminars by experts on novel and emerging methodologies on computational materials science, followed by essays written by the students on each seminar topic.
---

### 4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY.	Face-to-face
-----------	--------------

USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY			
TEACHING METHODS	<b>Activity</b>	<b>Semester workload</b>	
	Seminar lectures	39	
	Study and analysis of bibliography	41	
	Essay writing	70	
	Course total	<b>150</b>	
STUDENT PERFORMANCE EVALUATION	By evaluation of essays written during the course.		
	<b>General criteria for the assessment of students</b>		
	<p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course.</p>		

#### 5. RECOMMENDED BIBLIOGRAPHY

Books and scientific papers recommended by the speakers of the seminars related to the seminar topics.
--

## 3<sup>rd</sup> Semester

### Master Thesis II

#### COURSE OUTLINE

#### 1. GENERAL

SCHOOL	NATURAL SCIENCES		
ACADEMIC UNIT/PARTICIPATING UNITS	MATERIALS SCIENCE		
PARTICIPATING INSTITUTIONS			
POSTGRADUATE PROGRAMME: TITLE OF POSTGRADUATE PROGRAMME	Materials Science		
LEVEL OF STUDIES	Postgraduate		
COURSE CODE	EY-MT2	SEMESTER	3 <sup>rd</sup>
COURSE TITLE	Master Thesis II		
INDEPENDENT TEACHING ACTIVITIES	WEEKLY TEACHING HOURS	CREDITS	
	-	10	
COURSE TYPE	Specialised general knowledge		
PREREQUISITE COURSES:	NO		
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek or English if it is required		
IS THE COURSE OFFERED TO ERASMUS STUDENTS	YES		
COURSE WEBSITE (URL)	<a href="https://www.matersci.upatras.gr/el/studies/postgraduate/epistimi-tonylikon/msc-courses">https://www.matersci.upatras.gr/el/studies/postgraduate/epistimi-tonylikon/msc-courses</a>		

#### 2. LEARNING OUTCOMES

Learning outcomes
Conducting the second part of the Thesis (experimental or computational).
General Competences
<ul style="list-style-type: none"><li>- Search for, analysis and synthesis of data and information, with the use of the necessary technology - Adapting to new situations</li><li>- Working independently</li><li>- Team work</li><li>- Working in an international environment</li><li>- Working in an interdisciplinary environment</li><li>- Production of new research ideas</li><li>- Project planning and management</li><li>- Respect for the natural environment</li><li>- Criticism and self-criticism</li><li>- Production of free, creative and inductive thinking</li></ul>

### 3. SYLLABUS

Experimental of computational research work, writing and supporting in public of the Thesis
---

### 4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY	Face-to-face		
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY	Conducting experiments in the lab and data analysis or development and application of computational methods in materials science subjects.		
TEACHING METHODS	<i>Activity</i>	<i>Semester workload</i>	
	Conducting experiments/development,	350	
	use of computational methods		
	Data analysis, writing of the Master Thesis/public support of the Thesis.	400	
	<b>Course total</b>	<b>750</b>	

STUDENT PERFORMANCE EVALUATION	<p>Students are writing their Thesis and they supported in public in front of a three members committee.</p> <p style="text-align: center;"><b>General criteria for the assessment of students</b></p> <p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course. <b>General criteria for the assessment of students</b></p> <p><b>Written or oral examinations:</b> knowledge and understanding of the content of the course with development of theoretical topics and development/solution of relevant exercises-problems for the application of theory, ability to combine and synthesize concepts and develop a solution strategy.</p> <p><b>Studies and presentations or laboratory reports:</b> Structure and appearance, language, clarity and coherence, completeness of study and results processing, presentation of sources, presentation of work.</p> <p>The general assessment - grading criteria are accessible to students through the Student Guide. At the same time, they are specified by the teachers according to the nature of the course.</p>
--------------------------------	---

#### 5. RECOMMENDED BIBLIOGRAPHY

- *Suggested bibliography:*  
 Because of the nature of the course, specific bibliography cannot be recommended. - *Related academic journals:*