## **COURSE OUTLINE**

# (1) GENERAL

SCHOOL	School of Science				
ACADEMIC UNIT	Physics				
LEVEL OF STUDIES	Undergraduate				
COURSE CODE	10EK502		SEMESTER	7	
COURSE TITLE	PHYSICS OF MOLECULES AND NANOMATERIALS				
INDEPENDENT TEACHING ACTIVITIES if credits are awarded for separate components of the course, e.g. lectures, laboratory exercises, etc. If the credits are awarded for the whole of the course, give the weekly teaching hours and the total credits		WEEKLY TEACHING HOURS		CREDITS	
Lectures (theory and exercises)		4		6	
COURSE TYPE general background, special background, specialised general knowledge, skills development	Specialized				
PREREQUISITE COURSES:	No				
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek				
IS THE COURSE OFFERED TO ERASMUS STUDENTS	Yes, in the English language for Erasmus students				
COURSE WEBSITE (URL)	https://eclass.uoa.gr/courses/PHYS235/				

### (2) LEARNING OUTCOMES

#### Learning outcomes

The course learning outcomes, specific knowledge, skills and competences of an appropriate level, which the students will acquire with the successful completion of the course are described.

- Consult Appendix A
- Description of the level of learning outcomes for each qualifications cycle, according to the Qualifications Framework of the European Higher Education Area
- Descriptors for Levels 6, 7 & 8 of the European Qualifications Framework for Lifelong Learning and Appendix B
- Guidelines for writing Learning Outcomes

The course offers to the student the necessary knowledge for the understanding of basic concepts of physics of molecules and nanomaterials with emphasis on fundamental aspects of molecular bonding and molecular spectra as well as the electronic structure of nanomaterials (graphene and carbon nanotubes). With the completion of the course the student is able to:

- Apply the adiabatic Born-Oppenheimer approximation in order to determine the electronic structure of the hydrogen molecule-ion and hydrogen molecule using molecular orbital (linear combination of atomic orbitals –LCAO) and valence bond theories.
- Analyze the electronic structure (energy diagrams, bonding-antibonding molecular orbitals and terms, HOMO-LUMO, bond order and spin) of diatomic and polyatomic molecules and construct the sp<sup>n</sup> hybrid orbitals.
- Describe analytically nuclear motion (rotation, vibration) in diatomic molecules taking into account the effects of centrifugal distortion and anharmonicity and analyze the corresponding molecular spectra (rotational, vibrational and vibration-rotation) in order to calculate experimentally physical quantities of the molecules, such as the moment of inertia and equilibrium bond length.
- Distinguish the fine structure of electronic transitions due to vibrations-rotations and the spectral intensity variation based on the Franck-Condon principle.
- Apply the tight binding method to calculate the energy band structure of one-dimensional chain of atoms, polycatelyne and graphene (π and σ energy bands, linear energy dispersion relation, density of states).
- Describe the electronic band structure of carbon nanotubes (direct-reciprocal lattice, 1<sup>st</sup> Brillouin zone, zone folding-energy dispersion relation, metallic condition) classify them to metals and semiconductors according to their structural characteristics. Also, distinguish the density of states (Van Hove anomalies) of metallic and semiconducting nanotubes and the corresponding electronic transitions in relation to their diameter.

#### **General Competences**

Taking into consideration the general competences that the degree-holder must acquire (as these appear in the Diploma Supplement and appear below), at which of the following does the course aim?

Search for, analysis and synthesis of data and	Project planning and management
information, with the use of the necessary technology	Respect for difference and multiculturalism
Adapting to new situations	Respect for the natural environment
Decision-making	Showing social, professional and ethical responsibility and
Working independently	sensitivity to gender issues
Team work	Criticism and self-criticism
Working in an international environment	Production of free, creative and inductive thinking
Working in an interdisciplinary environment	
Production of new research ideas	Others

The course aims at the following general competences:

- Search for, analysis and synthesis of data and information, with the use of the necessary technology
- Working independently
- Analytical and synthetic thinking
- Critical thinking
- Problem solving

### (3) SYLLABUS

- Electronic structure of molecules. The hydrogen molecular ion: Method of linear combination of atomic orbitals. The hydrogen molecule: Molecular orbitals-valence bond method.
- Diatomic molecules: Homonuclear-heteronuclear. Polyatomic molecules. Delocalization. Hybridization.
- Nuclear motion of a diatomic molecule. Rotation. Vibration. Vibration-rotation. Molecular spectra. Raman effect. Electronic transitions: Franck-Condon principle.
- Tight binding method with many orbitals/unit cell. Electronic structure of polyacetylene. Graphene:  $\pi$  and  $\sigma$  energy bands, dispersion relation.
- Carbon nanotubes: Electronic structure (band folding, metallicity condition). Density of states. Energy transitions. Size effects.
- Imaging methods for nanomaterials: Atomic Force Microscopy (AFM), Scanning Tunneling Microscopy (STM), Scanning Near-field Optical Microscopy (SNOM).

# (4) TEACHING and LEARNING METHODS - EVALUATION

DELIVERY	Face-to-face				
, ace to jace, bistonice rearning, etc.	Live streaming (distance learning in special circumstances)				
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY Use of ICT in teaching, laboratory education, communication with students	Yes Electronic communication with the students using ICT (Information and Communications Technology) Computer-aided lectures, use of Overhead Projectors, eclass platform				
TEACHING METHODS	Activity	Semester workload			
The manner and methods of teaching are	Lectures	39			
described in detail. Lectures seminars laboratory practice	Tutorials	13			
fieldwork, study and analysis of bibliography,	Individual Study/ Study and	50			
tutorials, placements, clinical practice, art	Analysis of bibliography /				
workshop, interactive teaching, educational	Preparation				
etc.	Writing reports/ essays	45			
	Exams	3			
The student's study hours for each learning					
directed study according to the principles of the	Course Total 150				
ECTS					
STUDENT PERFORMANCE					
EVALUATION					
Description of the evaluation procedure	Final written exams in Greek (90%)				
Language of evaluation, methods of evaluation,	Writing essays (10%)				
summative or conclusive, multiple choice					
questionnaires, short-answer questions, open-					
essay/report, oral examination, public					
presentation, laboratory work, clinical					
examination of patient, art interpretation, other					
Specifically-defined evaluation criteria are					
given, and if and where they are accessible to					
students.					

### (5) ATTACHED BIBLIOGRAPHY

- Suggested bibliography:

- Notes «Introduction to Molecular Physics», M. Calamiotou, NKUA, 1992, Athens
- Molecular Quantum Mechanics, P.S. Atkins, Editions PAPAZISI, 1999, Athens
- Solid State Physics, H. Ibach, H. Luth, Editions P. & S. ZITI 2011, Thessaloniki
- M. Karplus, R. N. Porter, Atoms and Molecules: An Introduction for Students of Physical Chemistry, W. A. Benjamin, 1970.
- C. N. Banwell, Fundamentals of Molecular Spectroscopy, McGraw-Hill, 1994.
- R. Saito, M. S. Dresselhaus, G. Dresselhaus, Physical Properties of Carbon Nanotubes, London: Imperial College Press, 1998.
- S. Reich, C. Thomsen, J. Maultzsch, Carbon Nanotubes: Basic Concepts and Physical Properties, Wiley-VCH, Berlin, 2004.
- H. Rasa, Graphene Nanoelectronics. Metrology, Synthesis, Properties and Applications, Springer-Verlag Berlin Heidelberg 2012.