ETY910 - Introduction to advanced computational methods in materials science

COURSE OUTLINE

(1) GENERAL

SCHOOL	SCHOOL OF ENGINEERING		
ACADEMIC UNIT	DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING		
LEVEL OF STUDIES	UNDERGRADUATE		
COURSE CODE	ETY910	**SEMESTER**	6
COURSE TITLE	Introduction to advanced computational methods in materials science		

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	3	3
Add rows if necessary. The organization of teaching and the teaching methods used are described in detail at (d).		

COURSE TYPE *general background, special background, specialized general knowledge, skills development*	Special background, skills development
PREREQUISITE COURSES:	NO
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	GREEK
IS THE COURSE OFFERED TO ERASMUS STUDENTS	NO
COURSE WEBSITE (URL)	http://www.materials.uoi.gr/en/0,02,01.html

(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*

In the course, "Introduction to Advanced Computational Methods in Material Science" the student learns the modern computational theories that will enable him to study the atomic and electronic structure of a material using quantum mechanics. Starting from simple quantum mechanics problems, the course gradually proceeds to the complex materials' cases. The aim is to find the appropriate theories and approaches to describe the electronic structure of a material solving the Schrödinger's equation for a multi-particle system under constraints and conditions. These methods will allow the student to be able to calculate the structural, electrical, magnetic and optical properties of a material analytically or computationally through appropriate software.

Specifically at the end of the lesson the student should be able to:

- calculate the electronic structure of a crystal.
- calculate the energy eigenvectors and eigenvalues of a single molecule or its complexes.
- calculate the electronic structure of a periodic chain or a two-dimensional grid and investigating its metallic or semi-conductive or insulating behavior.

• calculate the magnetic moment of a material through the spin polarized electron density of states

• calculate the optical absorption of a molecule or semiconductor.

The active participation of students in exercises and problems and their further familiarity with the calculation programs in the computer plays an important role.

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 information, with the use of the necessary technology	*Project planning and management*
Adapting to new situations	*Respect for difference and multiculturalism*
Decision-making	*Respect for the natural environment*
Working independently	*Showing social, professional and ethical responsibility and 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…*
	…….

- Working independently
- Criticism and self-criticism
- Production of free, creative and inductive thinking
- Search for, analysis and synthesis of data and information, with the use of the necessary technology
- Team work

(3) SYLLABUS

The course "Introduction to Advanced Computing Methods in Material Science" contains:

1. Basic principles and problems of quantum mechanics.
   Schrödinger Equation, Square Well Potential, Periodic Square-Well Potential, Hydrogen atom
2. Introduction to ab initio calculations:
   Born-Oppenheimer approach, One-electron approach, Hartree method, Hartree-Fock method. Density Functional Theory. Augmented Plane Wave theory
3. Semi-Empirical Calculations:
   Linear Combination of Atomic Orbitals (LCAO) Theory of Tight Binding and Density Functional Binding Approach.
4. Applications in atomic and electronic structure calculations as well as predicting macroscopic properties of periodic systems, biological molecules and nanoscopic materials.

(4) TEACHING and LEARNING METHODS - EVALUATION

DELIVERY *Face-to-face, Distance learning, etc.*	In class, lectures
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY *Use of ICT in teaching, laboratory education, communication with students*	Electronic platform e-course

TEACHING METHODS
The manner and methods of teaching are described in detail.
Lectures, seminars, laboratory practice, fieldwork, study and analysis of bibliography,

Activity	***Semester workload***
Lectures	27
Fieldwork/Laboratory practice	12

tutorials, placements, clinical practice, art workshop, interactive teaching, educational visits, project, essay writing, artistic creativity, etc. *The student's study hours for each learning activity are given as well as the hours of non-directed study according to the principles of the ECTS*	Self-study/ project/essay writing	36
	Course total	75
STUDENT PERFORMANCE EVALUATION *Description of the evaluation procedure* *Language of evaluation, methods of evaluation, summative or conclusive, multiple choice questionnaires, short-answer questions, open-ended questions, problem solving, written work, 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.*	LANGUAGE OF EVALUATION: Greek METHOD OF EVALUATION: (i) Final written examination (ii) Public presentation	

(5) ATTACHED BIBLIOGRAPHY

-*Suggested bibliography*:

- Computational Physics II, A. Andrioths, 1999, Anikoyla press
- Solid State Physics E.N. Oikonomou, Crete University Press, 1997, Hrakleio

-Related academic journals: