ETE810 - Simulation and Materials Design Techniques

COURSE OUTLINE

(1) GENERAL

SCHOOL	SCHOOL OF ENGINEERING		
ACADEMIC UNIT	DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING		
LEVEL OF STUDIES	UNDERGRADUATE		
COURSE CODE	ETE810	**SEMESTER**	**10**
COURSE TITLE	Simulation and Materials Design Techniques		

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 and labs	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
PREREQUISITE COURSES:	NO
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	GREEK
IS THE COURSE OFFERED TO ERASMUS STUDENTS	NO
COURSE WEBSITE (URL)	http://pc164.materials.uoi.gr/dpapageo/courses/sim/

(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*

This is an introductory course in the concepts of classical atomic simulation. Upon completion of the course the student

Knowledge: Knows and understands the basic principles and theory of classical atomic simulation, the models used, the basic simulation methods as well as the corresponding scientific software.

Skills: Recognizes the main interactions in nature, selects the corresponding model and its parameters. Applies specialized scientific simulation software to calculate properties in metallic and organic systems

Ability: Is able to examine different systems using classical atomistic simulations, in different conditions, produce and interpret results related to their properties.

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…*
	…….

- Search, analyze and synthesize data and information, using the necessary technologies.
- Independent work
- Teamwork

(3) SYLLABUS

Models and interactions in classical atomistic simulation. Statistical ensembles (microcanonical, normal, isothermal/isobaric). The partition function. Thermodynamic properties. Molecular dynamics simulation. Newtonian dynamics. Equations of motion. Phase space. Fundamentals of Monte Carlo simulation. Metropolis criterion. Calculation of structural, thermodynamic and dynamic properties. Time correlation functions. Simulation software and applications in organic and inorganic systems.

(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*	By nature of the course, computers are used in the lab. In addition, specialized software is used to conduct laboratory exercises.
TEACHING METHODS *The manner and methods of teaching are described in detail. Lectures, seminars, laboratory practice, fieldwork, study and analysis of bibliography, 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*	

Activity	***Semester workload***
Lectures	26
Laboratory	13
Self-study (preparation for the final exam)	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*	LANGUAGE OF EVALUATION: Greek METHOD OF EVALUATION: Final written examination or project presentation.

to students.	

(5) ATTACHED BIBLIOGRAPHY

-Suggested bibliography: D. Papageorgiou. Computer Simulation methods, University of Ioannina, 2004.