

ETY506 - Atomic and electronic structure of solids

COURSE OUTLINE

(1) GENERAL

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| SCHOOL | SCHOOL OF ENGINEERING | | |
| ACADEMIC UNIT | DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING | | |
| LEVEL OF STUDIES | UNDERGRADUATE | | |
| COURSE CODE | ETY506 | SEMESTER | 5 |
| COURSE TITLE | Atomic and electronic structure of solids | | |
| INDEPENDENT TEACHING ACTIVITIES <i>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</i> | WEEKLY TEACHING HOURS | CREDITS | |
| Lectures | 4 | 4 | |
| <i>Add rows if necessary. The organization of teaching and the teaching methods used are described in detail at (d).</i> | | | |
| COURSE TYPE <i>general background, special background, specialized general knowledge, skills development</i> | General background | | |
| 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*

The primary objective of the course is to educate the student on the basic theories of the atomic and electronic structure of solids and gain experience in describing the crystalline structure and its relation to the electronic properties of a material. Particularly important is the understanding of the correlation of the chemical bond that will be developed between the electrons of the atoms and the final crystalline structure resulting therefore metallic, semiconductor or insulating properties. Because of this, students' active involvement in discussions concerning the correlation between the structure and the material's properties as well as problems' solving on the board throughout the semester plays an important role. The active participation of students in discussions and when solving problems in the black board are strongly supported.

At the end of the lesson the student should be able to:

- Actively involved in the teaching-learning process
- combines the crystal structure of an element with its position in the periodic table and the type of valence electrons.
- Describes the basic features of a crystal structure.

- Design the Brillouin zones and compare them with X-ray experiments
- Determines the electronic structure of a molecule and a one-dimensional solid by acquiring knowledge of its electrical, magnetic and optical properties.
- Paint the new hybrid orbital due to the interaction of metal ions with biological molecules to describe the potential antioxidant activity of the complex.
- Selects an element from the periodic table according to the type of its outer electrons and assumes its potential impact on the electrical properties of a material, for example the semiconductor energy gap for future technology applications in microelectronics.

Experience in the basic concepts and theories of Atomic and Electronic Structure of Materials will be the basis for the study of electrical, magnetic and optical properties of materials with various technological applications.

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?

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

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

(3) SYLLABUS

This course introduces to Atomic and Electronic Structure of Solids and the essential background required to follow the specialized topics that follow. The content of the course is as follows:

1. Periodicity and crystalline structure
Definitions and Theorems, Classification of Bravais Grids, Single Crystal Base, Simple and Complex Crystal Structures, Reverse Grid and Brillouin Zones.
2. "Building" crystals from individuals
Periodic Table, Periodic Table of Crystalline Structures, Individuals with External Shells, Individuals with External Electrons of Type s, Individuals with External Electrons of Type s and p, Hybrid orbitals sp² and sp³, Individuals with External Electrons of type s and d, Atoms electrons of type s, d and f, Bond types
3. Free electron model and Jellium model
Quantum Mechanics Basics, Schrödinger's Equation, Plane Waves, Free Electron in 1d and 3d Box, N Free Electrons in 1d and 3d Box, N Electron Gas in Periodic Box, Jellium Model, Electron Motion (Fermi wave, Energy electron kinetic energy and pressure). Electron density of states, Basic characteristics of solid matter. Ion motion in the Jellium model
4. Linear Atomic Combination Method
Introduction to the Linear Combination of Atomic Orbitals LCAO. Basic principles. LCAO parameters. Applications of the method and calculation of energy eigenvalues for: Hydrogen molecular ion, NaCl molecule and benzene molecule. LCAO in simplistic "solid" models. Calculation of the Electronic Structure of: Infinite one-dimensional

elemental "solid", One-dimensional ionic "solid" with one or two orbitals per atom and Periodic one-dimensional arrangement of similar atoms. Electronic structure of a magnetic material.

5. Introduction to Semiconductors

Crystalline Structure and Characteristics of Semiconductors, Electronic Semiconductor Structure, Direct and Indirect Gap Semiconductors. Optical absorption and coupling to the electronic structure of a material. Excitons (characteristics, properties and categories).

(4) TEACHING and LEARNING METHODS - EVALUATION

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|---|--|--------------------------|
| DELIVERY <i>Face-to-face, Distance learning, etc.</i> | In class, lectures | |
| USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY <i>Use of ICT in teaching, laboratory education, communication with students</i> | Electronic platform e-course | |
| TEACHING METHODS <i>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</i> | Activity | Semester workload |
| | Lectures | 39 |
| | Fieldwork | 13 |
| | Self-study | 48 |
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| | Course total | 100 |
| STUDENT PERFORMANCE EVALUATION <i>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.</i> | <p>LANGUAGE OF EVALUATION: Greek</p> <p>METHOD OF EVALUATION:</p> <p>(i) Final written examination</p> | |

(5) ATTACHED BIBLIOGRAPHY

-Suggested bibliography:

- Solid State Physics E. N. Ουκοβοπου, Crete University Press, 1997, Hrakleio
- Solid State Physics, Ashcroft Mermin, Press: (A. G. Πνευματικός)

-Related academic journals: