ΜΟΝΑΔΑ ΔΙΑΣΦΑΛΙΣΗΣ ΠΟΙΟΤΗΤΑΣ Α.Π.Θ.

6th Semester

Design of materials in the atomic scale

1. GENERAL			
SCHOOL	Faculty of Sciences in collaboration with Faculty of Engineering, Aristotle University of Thessaloniki		
DEPARTMENT	Materials Science and Engineering		
LEVEL OF STUDIES	ISCED level 7 (5-year Integrated Master's programme) ISCED level 6 (4-year BSc programme)		
COURSE CODE	**MSEN 601**	SEMESTER	6th Semester
COURSE TITLE	**Design of materials in the atomic scale**		
TEACHING ACTIVITIES Lectures, tutorials/problem sessions, laboratory/computer exercises (where applicable), case studies and guided self-study.		TEACHING HOURS PER WEEK	ECTS CREDITS
		4	6
COURSE TYPE	This course introduces the principles and techniques for designing and understanding materials at the atomic and molecular level. Topics include atomic structure, bonding, crystal structures, defects, and computational modeling methods used to predict and tailor material properties. Emphasis is placed on linking atomic-scale phenomena to macroscopic material behavior, enabling students to design materials with desired mechanical, electronic, thermal, and chemical properties for advanced engineering applications.		
PREREQUISITES	This course builds on foundational knowledge in materials science, solid-state physics, chemistry, and crystallography. Students are expected to understand atomic structure, bonding, crystal lattices, and basic thermodynamics. Familiarity with computational methods or software for modeling atomic-scale systems is helpful but not required, as the course introduces relevant simulation and analysis techniques.		
TEACHING AND EXAMINATION METHODS	Lectures, Homework assignments, Quizzes, Midterm examination, Final exam		
COURSE OFFERED TO ERASMUS STUDENTS	Yes.		
COURSE URL	https://elearning.auth.gr/course/view.php?id=xxxxx		

2. LEARNING OUTCOMES	
Learning Outcomes	Upon successful completion of the course, students will be able to: ● Explain atomic and molecular structure, bonding, and crystal arrangements in materials. ● Analyze the role of defects and atomic-scale phenomena in determining material properties. ● Apply computational modeling and simulation techniques to predict material behavior at the atomic scale. ● Relate atomic-level design decisions to macroscopic mechanical, thermal, electronic, and chemical properties. ● Integrate theoretical knowledge and practical methods to design

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<tr><td></td><td>materials for specific engineering applications.
● Communicate atomic-scale materials design concepts clearly using written, graphical, and oral forms.</td></tr>
<tr><td>General Skills</td><td>Upon completing this course, students will develop the following skills:
General Skills
1. Analytical Thinking: Ability to analyze atomic-scale structures and relate them to material properties.
2. Problem-Solving: Design materials with specific properties using theoretical and computational methods.
3. Research Skills: Evaluate scientific literature and apply advanced concepts to materials engineering problems.
4. Engineering Application: Translate atomic-scale understanding into practical materials solutions.
Soft Skills
1. Communication: Present scientific results clearly in written, graphical, and oral formats.
2. Teamwork: Collaborate effectively in laboratory, simulation, or project-based group activities.
3. Critical Thinking: Assess design decisions and interpret computational and experimental results.
4. Time Management: Plan and execute projects and assignments efficiently.
Adaptability and Lifelong Learning: Apply knowledge to new materials challenges and stay updated with emerging techniques</td></tr>
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3. COURSE CONTENT

This course covers the principles of atomic and molecular structure, bonding, crystal structures, and defects, emphasizing their influence on material properties. Students learn computational modeling and simulation techniques to predict material behavior and apply atomic-scale design strategies to develop advanced materials for engineering applications. Course content includes:

1. **Atomic Structure and Bonding, Crystal Structures and Defects**
2. **Materials Properties at the Atomic Scale**
   - Mechanical, thermal, electronic, and optical behavior
   - Role of atomic arrangement in determining macroscopic properties
   - Structure–property relationships
3. **Computational Modeling and Simulation**
   - Molecular dynamics and Monte Carlo simulations
   - Density functional theory basics
   - Predicting material behavior and guiding design decisions
4. **Materials Design Strategies**
   - Tailoring atomic structure for desired properties
   - Design of alloys, composites, and nanostructured materials
   - Case studies of engineered materials
5. **Applications in Materials Engineering**
   - Advanced functional materials
   - Nanoengineered materials and devices

Linking atomic-scale design to industrial applications

4. LEARNING & TEACHING METHODS - EVALUATION

Teaching method	Face-to-face.

<table>
<tr><td>Use of ICT</td><td>ICT plays a significant role in enhancing teaching, learning, experimentation, visualization, and assessment in this course as follows:
Computational Tools for Problem Solving: Spreadsheet calculations (Excel, Google Sheets), Coding solutions in Python, MATLAB, or Mathematica
Online Learning Platforms: Learning management systems (LMS) like Moodle, Online lectures, video tutorials, and animations,
Communication and Collaboration: Online discussion forums, Collaborative documents, Sharing of data and reports
Presentation and Reporting Tools: Lab reports (word processors), Data plots and charts (graphing tools), Presentations (PowerPoint, Google Slides).</td></tr>
<tr><td>Teaching organization</td><td>The supervised and unsupervised workload per activity is indicated below (total workload complies with ECTS standards).
<table><tr><th>Activity</th><th>Workload/semester (hours)</th></tr><tr><td>Lectures</td><td>52</td></tr><tr><td>self-study, quizzes, on-line tests</td><td>46</td></tr><tr><td>Independent study</td><td>50</td></tr><tr><td>Final written exam</td><td>2</td></tr><tr><td>Total</td><td>150</td></tr></table></td></tr>
<tr><td>Student evaluation</td><td>Assessment Language: English
• Assessment Methods: Multiple Choice Test, Short Answer Questions, Essay Development Questions, Problem Solving, Written Assignment, Written Exams</td></tr>
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5. SUGGESTED BIBLIOGRAPHY

Course Bibliography

Materials Interfaces | ISBN 978-0-412-41270-7 | Springer 1992

Additional bibliography for study

Materials and Design: The Art and Science of Material Selection in Product Design | ISBN | Butterworth-Heinemann 2014