COURSE OUTLINE

(1) GENERAL INFORMATION

SCHOOL	SCHOOL OF APPLIED MATHEMATICAL AND PHYSICAL SCIENCES		
DEPARTMENT	SCHOOL OF APPLIED MATHEMATICAL AND PHYSICAL SCIENCES		
LEVEL OF STUDIES	POSTGRADUATE		
MSc PROGRAM	MICROSYSTEMS AND NANODEVICES		
COURSE CODE	**9960**	**SEMESTER**	**2**
COURSE TITLE	SIMULATION AT THE MICRO- AND MACRO-LEVEL		

INDEPENDENT TEACHING ACTIVITIES *In cases where credits are awarded to discrete parts of the course (e.g., Lectures, Laboratory Exercises, etc.), specify them. If credits are awarded as a whole, specify weekly teaching hours and total credits.*	**WEEKLY TEACHING HOURS**	**ECTS**
Lectures – Exercises	3	6
Laboratory	0	
Assignments	0	
(Additional rows may be added if necessary. Detailed descriptions of teaching organization and methods are provided in section (d).)		

COURSE TYPE *general background, specialized background, specialization, skill development*	SPECIALIZATION (for Streams or Specialization Compulsory courses)
PREREQUISITES:	[REQUIRED BACKGROUND KNOWLEDGE]: Physics (Mechanics), Differential and Integral Calculus, Probability Theory, Basic Undergraduate-Level Computer Programming
LANGUAGE OF INSTRUCTION and EXAMINATION:	GREEK
COURSE AVAILABLE TO ERASMUS STUDENTS	YES (offered in English as a reading course).
COURSE WEBSITE (URL)	https://helios.ntua.gr/course/view.php?id=3016

(2) LEARNING OUTCOMES

Learning Outcomes

This section describes the learning outcomes of the course, specifying the knowledge, skills, and competencies at the appropriate level that students will acquire upon successful completion of the course.

Refer to Appendix A:

- *Description of the Level of Learning Outcomes for each cycle of studies according to the European Higher Education Area Qualifications Framework*
- *Descriptive Indicators for Levels 6, 7, & 8 of the European Qualifications Framework for Lifelong Learning and Appendix B.*
- *Concise Guide to Writing Learning Outcomes*

Knowledge:

Modeling and computational simulation at the molecular, mesoscale, and macroscopic levels have become essential tools for understanding the structure-property-processing-performance relationships of materials and designing products that meet specific application requirements. Building on this premise, the course objectives are:

- To familiarize students with the principles of statistical mechanics for systems within and outside of thermodynamic equilibrium.
- To provide guidelines for developing microscopic and mesoscopic material models for theoretical analysis and simulation.
- To understand the fundamental principles and applications of stochastic (primarily Monte Carlo) and deterministic (primarily Molecular Dynamics) computational simulation methods for predicting material properties.

- To practice computational methods for characterizing material structure and molecular mobility, linking results to experimental measurements.

Skills:

Upon successful completion of the course, students will be able to:

- Apply the principles of statistical mechanics to express thermodynamic (e.g., volumetric behavior, enthalpy, chemical potential), dynamic (e.g., diffusion coefficients, viscosity, thermal conductivity), and mechanical (e.g., stress, elastic constants) properties of a material system as equilibrium ensemble averages.
- Understand how structure and dynamics in a material system can be quantitatively described via spatial and temporal correlation functions and how these descriptions can be validated through scattering or spectroscopy experiments.
- Select appropriate force fields for describing material systems at the atomic level.
- Use computational Monte Carlo or molecular dynamics codes to perform molecular simulations of materials.
- Analyze simulation results to extract properties and reveal the molecular mechanisms underlying them.
- Grasp the principles of systematic coarse-graining of molecular representations and mesoscale simulation methods (e.g., Langevin Dynamics, Brownian Dynamics, Dissipative Brownian Dynamics) to study material systems at extended length and time scales and predict their properties.
- Understand the principles of rare event theory and its applications for predicting phenomena such as diffusion, structural relaxation, nucleation, and growth.
- Devise strategies for simulating materials across multiple length and time scales as a means of molecular material design.

General Competencies

Considering the general competencies that graduates are expected to acquire (as stated in the Diploma Supplement), which competencies does this course aim to develop?.

Data search, analysis, and synthesis, utilizing necessary technologies	*Generation of new research ideas*
Adaptability to new situations	*Project design and management*
Decision-making	*Respect for diversity and multiculturalism*
Independent work (primarily through assignments completed at home)	*Respect for the natural environment*
Teamwork	*Exhibiting social, professional, and ethical responsibility and sensitivity to gender issues*
Working in an international environment	*Critical and self-critical thinking*
Working in an interdisciplinary environment	*Promotion of free, creative, and inductive thinking*

Competencies:

Upon successful completion of the course develops the ability to:

- Work independently (and, secondarily, in teams through assigned group projects).
- Search for, analyze, and synthesize data and information using computational technologies.
- Formulate a physical/scientific/technological problem in mathematical terms.
- Design workflows that employ computational methodologies at various levels (atomistic, mesoscale, macroscopic), according to the length and time scales relevant to a given problem.

- Combine knowledge and skills: (a) to analyze a complex problem, or (b) to select appropriate tools, methods, and approaches for designing materials for specific applications.

(3) COURSE CONTENT

I. Principles of Statistical Mechanics

Dynamical trajectories in phase space. Probability density of a statistical ensemble. Liouville equation. Irreversibility and attainment of thermodynamic equilibrium. Equilibrium statistical ensembles: microcanonical, canonical, isothermal-isobaric. Calculation of thermodynamic properties. Pressure (stress) as an equilibrium ensemble average: the virial theorem. Chemical potential as an equilibrium ensemble average: Widom's theorem. Grand canonical ensemble for open systems: density fluctuations, calculation of sorption isotherms. Distribution functions for characterizing structure, their relation with thermodynamic properties and with X-ray and neutron diffraction measurements.

II. Molecular simulations

Molecular models and force fields, periodic boundary conditions. Computation of the total potential energy. Monte Carlo integration, Monte Carlo sampling. Connection with the theory of stochastic processes. Metropolis algorithm in the canonical, isothermal-isobaric and grand canonical ensembles. Bias in attempting elementary moves and corresponding acceptance rules. Molecular dynamics simulations. Algorithms for integrating the equations of motion. Molecular dynamics in the presence of holonomic constraints dictated by molecular geometry. Molecular dynamics in statistical ensembles other than the microcanonical. Analysis of molecular simulation trajectories for the determination of structural, thermodynamic, and dynamical properties. Time correlation functions and their relation with spectroscopic measurements. Elements of linear response theory. Computation of transport coefficients (diffusivity, thermal conductivity, viscosity).

III. Techniques for long time and length scales

Coarse-graining and reduction to models with fewer degrees of freedom for the study of phenomena at long time and length scales. Projection of the equations of motion onto few, slowly evolving degrees of freedom. Elements of Brownian motion theory. Principles of Brownian Dynamics and Dissipative Particle Dynamics. Transition-state theory for estimating the rates of infrequent events. Kramers equation for the rate constant. Bennett-Chandler theory for determining the rate constant from molecular simulation. Computation of transition paths and rate constants with many, coupled, slowlyevolving degrees of freedom. Poisson processes resulting from successions of infrequent events. Master equation. Kinetic Monte Carlo simulation.

IV. Applications

Discussion of examples of molecular simulation work aiming at understanding and prediction of structure, thermodynamic and rheological properties of long-chain polymer melts; permeability of polymer membranes; structure and function of lipid bilayer membranes and biological macromolecules; self-organization phenomena in copolymers; polymers at interfaces; sorption and diffusion in zeolites; structural relaxation and mechanical properties in the glassy state; thin films, nanoparticles and nanocomposite materials.

(4) TEACHING AND LEARNING METHODS - ASSESSMENT

TEACHING METHOD *In person, Distance Learning etc.*	In person
USE OF INFORMATION AND COMMUNICATION TECHNOLOGIES (ICT) *Use of Information and Communication Technologies (ICT) in Lecturing, Laboratory Training, Communication with Students*	Course Notes, Assignments for Home Study **(**Assignments are provided by the lecturer, and students are required to submit completed work)
ORGANIZATION OF TEACHING *A detailed description of the teaching methods and approaches used in the course, which may include:* *Lectures, Seminars, Laboratory Exercises, Fieldwork, Study and Analysis of Bibliography, Tutorials, Internships, Clinical Exercises, Art Workshops, Interactive Teaching, Educational Visits, Project Development, Report Writing/Assignments, Artistic Creation.* *The student's study hours for each learning activity, as well as hours of independent study, are outlined in accordance with ECTS principles.*	

Activity	***Semester Workload***
Lectures	13x3=39 hours
Study	13x4=52 hours
Home Assignments/Exercises	2x20=40 hours
Laboratory	
Completion/Presentation of Project	1x30=30 hours
Educational Visits	0
Examinations	
Total Course Load	161

STUDENT ASSESSMENT *Description of the Assessment Process* *Language of Assessment, Assessment Methods, Formative / Summative Assessment Methods, Multiple-choice tests, Short-answer questions, Essay-style questions, Problem-solving exercises, Written assignments, Reports, Oral examinations, Public presentations, Laboratory work, Clinical patient examinations, Artistic interpretations, Other methods, as appropriate* *The assessment criteria are clearly defined and provided to students, ensuring transparency in the evaluation process. These criteria are accessible through the course's online platform where students can review them at any time.*	Language of Assessment: Greek (for Erasmus students: English) Two sets of computational exercises: 2 x 30% = 60% of the final grade Computational project (Monte Carlo or molecular dynamics, undertaken by pairs): 40% of the final grade These assessment criteria are explicitly outlined in the course introduction and in the posted problem statements on the Helios system.

(5) RECOMMENDED BIBLIOGRAPHY

Recommended Bibliography

Lecturer's Notes (posted on Helios platform):

- ***D.N. Theodorou, "Applied Molecular Theory for Engineers" (in English)***

Copies of Lecture Slides (in Greek)

Recommended Books from International Literature:

- ***D. Frenkel and B. Smit, "Understanding Molecular Simulation: From Algorithms to Applications," Academic Press: New York, 2002.***
- ***M.P. Allen and D.J. Tildesley, "Computer Simulations of Liquids," Clarendon Press: Oxford, 1989.***
- ***A.R. Leach, "Molecular Modelling: Principles and Applications," Pearson-Prentice Hall: London, 2001.***
- ***P. Nielaba, M. Mareschal, G. Ciccotti, "Bridging Time Scales: Molecular Simulations for the Next Decade," Springer: Berlin, 2002.***
- ***D. Chandler, "Introduction to Modern Statistical Mechanics," Oxford University Press: Oxford, 1987.***