

BIOPHAM Master - Syllabus of the courses proposed at the University of Pisa (UNIFI)

Course name	QUANTUM PHYSICS OF MATTER		
Credit Points (ECTS) 6	Workload (Face-to Face) 48	Duration 1 semester	Offered (Term) 1
Institution in charge	University of Pisa		
Instructors	Giuseppe Carlo La Rocca		
Purpose of the module	BIOPHAME Track	Mode	
	All tracks	Compulsory (Recommended for for students with no “quantum mechanics” background)	
Contents	<p><i>Introduction to quantum mechanics:</i> Waves and particles. Wave-particle duality and uncertainty principle. Wave function. Schroedinger equation and stationary states. Expectation values.</p> <p><i>Atomic Physics:</i> First atomic models and their shortcomings. Hydrogen atom: energy spectrum, angular momentum and eigenfunctions. Electron spin. Pauli exclusion principle. Helium atom, singlet and triplet states. Many-electron atoms, periodic system of elements. Atomic spectroscopy.</p> <p><i>Molecular physics:</i> Adiabatic approximation. The ionized hydrogen molecule. The hydrogen molecule. Homonuclear and heteronuclear diatomic molecules. Polyatomic molecules. Molecular vibrations. Molecular Spectroscopy.</p> <p><i>Condensed matter physics:</i> Structure of liquids, amorphous solids and crystals. X-ray diffraction. Types of crystals: molecular, ionic, covalent and metallic. Boltzmann distribution, equipartition of energy. Quantum statistics: bosons and fermions. Phonons and specific heat of solids. Free electron model of metals: electrical conductivity and specific heat.</p>		
Examination	Oral exam		
Requirement for examination	Conceptual and practical knowledge on quantum mechanics and its relation to the behavior of atoms, molecules and solids.		
More information	CLASSIFICATION: PHYSICS		
Learning outcomes	On successful completion of the course students will be familiar with the basic concepts and methods of nonrelativistic quantum mechanics which are at the base of the modern theory of atoms, molecules and condensed matter systems. He/she will also be able to peruse the literature on the quantum microscopic theory of matter that might be useful for his/her studies/research/work.		

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Course name	SOLID STATE PHYSICS 1		
Credit Points (ECTS) 6	Workload (Face-to Face) 48	Duration 1 semester	Offered (Term) 1
Institution in charge	University of Pisa		
Instructors	Stefano Roddaro		
Purpose of the module	BIOPHAME Track	Mode	
	All tracks	Compulsory (Recommended for for students with "quantum mechanics" background)	
Contents	<p>Electrons in a one-dimensional periodic potential. Electron tunneling through a periodic potential. Velocity, quasimomentum and effective mass of an electron in a band. Geometric description of crystals: direct and reciprocal lattices. Von Laue and Bragg scattering. The Drude electron gas. The theory of Sommerfeld. Energy and density of states of a two-and three-dimensional electron gas in a magnetic field. De Haas van Alphen effect. Landau diamagnetism and Pauli paramagnetism. Theory of harmonic crystal. Phonons. Optical properties of semiconductors and insulators. Charge transport in intrinsic and doped semiconductors. Fermi level in intrinsic semiconductors. Law of mass action. Donor and acceptor levels. Fermi level in doped semiconductors.</p>		
Examination	Oral Exam		
Requirement for examination			
More information	CLASSIFICATION: PHYSICS		
Learning outcomes	<p>On successful completion of the course students will be able to interpret the main experimental phenomenology of condensed matter - will obtain a sound knowledge of structural, electronic, optical and vibrational properties of solids.</p>		

Course name	DISORDERED AND OFF-EQUILIBRIUM SYSTEMS		
Credit Points (ECTS) 6	Workload (Face-to Face) 48 hours	Duration 1 semester	Offered (Term) 1
Institution in charge	University of Pisa		

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Instructors	Simone Capaccioli	
Purpose of the module	BIOPHAME Track	Mode
	All tracks	compulsory
Contents	<p><i>1. From order to disorder</i></p> <p>Non-periodical Long range positional order: quasi-crystals Disorder in long range positional atomic systems (cellular disorder): Substitutional disorder: interstitial and substitutional impurities, vacancies; Orientational disorder: plastic crystals (e.g. fullerene) Disorder in atomic systems without long range positional order (topological disorder): Base elements in real crystals: Dislocations and Burger's vector, Interfacial defects. Liquid state and amorphous state: N-bodies distribution functions, particular case: pair distribution; static structure factor; Hard sphere atomic liquids: Percus-Yevick theory. Disorder in polymeric systems: Conformations of polymeric linear chain: analogy with random walk. Chain rigidity: Kuhn's segment. Size distribution of linear polymeric chain. Free energy of polymeric chain, entropic elasticity. Pair distribution function of polymeric chain: self-similarity</p> <p><i>2. From equilibrium to out of equilibrium</i></p> <p>Supercooled metastable states and glass transition in liquids: Van Hove function and its momenta; Collective and microscopic dynamics: cage effect and vibrational properties, local and structural relaxation, relaxation time distribution, diffusion, visco-elasticity; Simple models of glass transition: Free volume, Configurational entropy. Elements of non-equilibrium thermodynamics: Zero Principle: fictive temperature in glasses, fluctuation-dissipation theorem violation; Second Principle: Jarzynski's equality and Crooks fluctuation theorem: experimental tests in nanosystems. Polymeric chain Dynamics: Short chain: Rouse model; Long chain: entanglement effect; Edwards tube model; De Gennes reptation motion: scale arguments. Non-equilibrium states in active matter: Molecular Motors; Bacteria, Swimmers, swarms: emergent collective motions and glass transition.</p> <p><i>3. Experimental techniques: structure and dynamics of disordered systems</i></p> <p>Scattering from disordered systems: generalities: Scattering cross sections, coherent and incoherent scattering; Static and dynamic structure factor, elastic and inelastic scattering; Spatial, temporal and spatio-temporal correlation function. Photon Scattering (X-rays and light): Sources of coherent radiation (synchrotron), spectrometers and detectors; Structure of disordered systems: X-ray diffraction at wide and small angle; Dynamics in disordered systems: Brillouin and Raman scattering, inelastic X-ray scattering, photocorrelation spectroscopy. Neutron scattering: Neutron sources and detectors: typical experimental layout; Structure of disordered systems: neutron diffraction at wide and small angle, comparison with X-ray; inelastic neutron scattering and spectroscopy: TAS, TOF, Backscattering, Spin-Echo.</p>	

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Examination	Knowledge will be assessed via: ongoing assignments and final oral exam.
Requirement for examination	
More information	CLASSIFICATION: PHYSICS
Learning outcomes	On successful completion of the course students will be able to understand and analyse scientific reports concerning experimental, theoretical and computational studies concerning the physics of disordered and off-equilibrium systems.

Course name	MECHANICAL BEHAVIOUR OF MATERIALS		
Credit Points (ECTS) 6	Workload (Face-to Face) 48 hours	Duration 1 semester	Offered (Term) 1
Institution in charge	University of Pisa		
Instructors	Andrea Lazzeri		
Purpose of the module	BIOPHAME Track	Mode	
	All tracks	compulsory	
Contents	<p>1. Introduction to deformation behaviour: Concept of stresses and strains, engineering stresses and strains, Different types of loading and temperature encountered in applications.</p> <p>2. Tensile Test - stress-strain response for metal, ceramic and polymer, elastic region, yield point, plastic deformation, necking and fracture.</p> <p>3. Bonding and Material Behaviour, theoretical estimates of yield strength in metals and ceramics.</p> <p>4. Elasticity (the State of Stress and strain, stress and strain tensor, tensor transformation, principal stress and strain, elastic stress-strain relation, anisotropy, elastic behaviour of metals, ceramics and polymers).</p> <p>5. Viscoelasticity (Molecular foundations of polymer viscoelasticity. Rouse-Bueche theory, Boltzmann superposition principle, mechanical models, distribution of relaxation and retardation times, interrelationships between mechanical spectra, the glass transition, secondary relaxations, dielectric relaxations.</p>		

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	<p>6. Plasticity (Hydrostatic and Deviatoric stress, Octahedral stress, yield criteria and yield surface, texture and distortion of yield surface, Limitation of engineering strain at large deformation, true stress and true strain, effective stress, effective strain, flow rules, strain hardening, Ramberg-Osgood equation, stress-strain relation in plasticity, plastic deformation of metals and polymers).</p> <p>7. Microscopic view of plastic deformation: crystals and defects, classification of defects, thermodynamics of defects, geometry of dislocations, slip and glide, dislocation generation - Frank Read and grain boundary sources, stress and strain field around dislocations, force on dislocation - self-stress, dislocation interactions, partial dislocations, twinning, dislocation movement and strain rate, deformation behavior of single crystal, critical resolved shear stress (CRSS), deformation of poly-crystals, Hall-Petch and other hardening mechanisms, grain size effect - source limited plasticity, Hall-Petch breakdown, dislocations in ceramics and glasses. Effects of microstructure on the mechanics of polymeric media: deformation modes, yield, rubber toughening, alloys and blends.</p> <p>8. Fracture mechanics (energetics of fracture growth, plasticity at the fracture tip, measurement of fracture toughness, - Linear fracture mechanics -KIC. Elasto-plastic fracture mechanics - JIC, Measurement and ASTM standards, Design based on fracture mechanics, effect of environment, effect of microstructure on KIC and JIC. Application of fracture mechanics in the design of metals, ceramics, polymers and composites, damage tolerance design, elements of fractography)</p> <p>9. Fatigue (S-N curves, low- and high-cycle fatigue, laboratory testing in fatigue, residual stress, surface and environmental effects, fatigue of cracked components, designing out fatigue failure, Life cycle prediction, Fatigue in metals, ceramics, polymers and composites.</p> <p>10. Creep. Creep in crystalline materials (stress-strain-time relationship, creep testing, different stages of creep, creep mechanisms and creep mechanism maps, diffusion, creep and stress rupture, creep under multi-axial loading, microstructural aspects of creep and design of creep resistant alloys, high temperature deformation of ceramics and polymers.</p>
<p>Examination</p>	<p>Knowledge will be assessed via: ongoing assignments and final oral exam.</p>
<p>Requirement for examination</p>	<p>Knowledge of the mechanical behaviour of a wide variety of materials ranging from conventional metals and alloys, ceramics and polymers to hybrid materials and biomaterials, at different length and time scales, from the continuum description of properties to the atomistic and molecular mechanisms that confer those properties to all materials. Knowledge of the micro-mechanics of deformation of metals, ceramics, polymers and composites. Knowledge of the fundamentals of elasticity and viscoelasticity, plasticity, imperfections/defects in crystals, deformation and strain-hardening, fracture, strengthening of alloys, martensitic transformations,</p>

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	intermetallics and foams, creep and superplasticity, fatigue.
More information	CLASSIFICATION: MATERIALS SCIENCE
Learning outcomes	<p>After the completion of the course, the students will be able to:</p> <ul style="list-style-type: none"> -understand the mechanism of plastic deformation and origin of materials strength; -suggest ways by which engineering materials may be intrinsically strengthened; - derive ductile-brittle transition temperature and select materials accordingly; - understand high temperature mechanical behavior of materials and be able to select the materials for high temperature applications; - design and select engineering components based on the principles of fracture mechanics and fatigue; -improve materials resistance to fracture and fatigue performance.

Course name	POLYMER SCIENCE AND ENGINEERING		
Credit Points (ECTS) 6	Workload (Face-to Face) 48 hours	Duration 1 semester	Offered (Term) 1
Institution in charge	University of Pisa		
Instructors	Giuseppe Gallone		
Purpose of the module	BIOPHAME Track	Mode	
	All tracks	Optional	
Contents	<p>Introduction to the course. Subject, tentative program, goals. Introductory survey on the universe of polymers, classification in plastics and elastomers, recyclable and not recyclable polymers. Historical milestones of polymer science and engineering.</p> <p>Basic review of general concepts in polymer science. Molecular structure, homo- and co-polymers, functionality of a monomer, possible skeletal configurations: linear, branched and crosslinked polymers. Classification of polymers as thermoplastics, elastomers and thermosets. Semi-crystalline and amorphous thermoplastics. Melting and glass transition. Survey on the typical values of properties (mechanical, electrical, density, thermal stability) of most employed thermoplastics, thermosets and elastomers.</p>		

	<p>Deformation mechanisms acting in polymers at the microscopic scale and factors that influence the mechanical response. Viscoelasticity of polymers. Molecular weight, molar masses and degree of polymerization.</p> <p>Generalities of step-growth polymerization. Linear step polycondensation and polyaddition reactions. Control of degree of polymerization in step-growth reactions: Carothers theory and statistical analysis. Kinetics of step polymerization and methods for controlling reactions. Network step polyaddition. Gelation: significance, problems in the quantitative definition of the gel-point, consequences at microscopic and macroscopic scales. Carothers theory and Flory theory of gelation. Brief mention about dendrimers and hyperbranched polymers.</p> <p>Generalities of chain-growth polymerizations. Stages of a linear chain-growth polyaddition. Production of free radicals activators by thermolysis, photolysis and redox reactions. Propagation stage. Termination by combination and disproportionation. Termination by intra- and inter-molecular chain transfer. Kinetics of linear chain polyadditions and steady state conditions. Degree of polymerization. Diffusion constraints and diffusion controlled reactions. Autoacceleration. Effects of chain transfer. Molar mass distribution. Effects of temperature. Ceiling temperature. Industrial methods for polymerization: bulk, solution, suspension and emulsion processes. Network radical polymerization by crosslinking monomers. Network radical polymerization of unsaturated (pre-)polymers.</p> <p>Thermodynamics of ideal solutions. Liquid lattice, Gibbs free-energy for mixing, configurational entropy. The Flory-Huggins theory and its limitations. Chemical potential. Dilute polymer solutions. The cohesive density approach for predictions of polymer solubility. Chain dimensions: the freely-jointed chain model, bond angle constraints and short-range steric restrictions, stiffness of a polymer chain. Long-range steric interactions and chains with excluded volume. Expansion parameters for the end-to-end distance and for the gyration radius of a polymer molecule coil. Frictional properties of polymers in solutions. Free-draining and non-draining regimes. Hydrodynamic volume and intrinsic viscosity of a polymer in solution in the non-draining limit: the Flory-Fox and the Mark-Houwink-Sakurada equations. Diffusion process in the non-draining limit. Behaviour of polyelectrolytes in solution.</p> <p>Characterization of polymers at molecular level. Techniques for measuring the number average molar mass based on colligative effects. Membrane osmometry. Vapour pressure osmometry. Ebulliometry and cryoscopy. End-group analysis. Scattering methods for characterization of polymers: static light scattering by liquids and solutions of small molecules and scattering by large molecules in solution. Effect of molar mass dispersity. The Zimm-</p>
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	<p>plot method for analysis of data. Dynamic light scattering. Photon correlation spectroscopy. Small-angle X-ray and neutron scattering. Purposes, limits and methods for SAXS and SANS analysis.</p> <p>Measurement of frictional properties of polymers in solutions. Dilute solution viscometry. The intrinsic viscosity, the Huggins equation for the reduced viscosity and the Kraemer equation for the inherent viscosity. Determination of average molar mass and expansion parameter for polymer molecules in solutions. Use of capillary viscometers for measuring the relative viscosity of a polymer in solution. Differential viscometer.</p> <p>Molar mass distribution. Fractionation of dilute Polymer Solutions by Phase-Separation. Gel permeation chromatography: separation by size exclusion, GPC calibration and data analysis, universal calibration for GPC. Porous gels and eluants for GPC. Instrumentation and procedures for GPC. Mass spectroscopy (MS). Mass spectra of polymers. ESI and MALDI methods for soft ionization. Time-of-flight (ToF) mass spectroscopy. Analysis of MALDI-TOF mass spectra of polymers. Use of MALDI MS for examining the chemical structure of polymers.</p> <p>Spectroscopic methods for characterization of chemical composition and molecular microstructure of polymers. The principles of spectroscopy and the Lambert-Beer law. Principles of UV-vis spectroscopy, applications in polymer science, essential apparatus and experimental procedures. Principles of IR spectroscopy, applications in polymer science, apparatus and experimental procedures, interpretation of IR spectra. Principles of Raman spectroscopy, applications in polymer science, interpretation of Raman spectra. Brief mention about Raman microscopy. Principles of NMR spectroscopy, interpretation of NMR spectra, absorption splitting by J-coupling. Applications of NMR spectroscopy in polymer science.</p> <p>The amorphous state of polymers. The glass transition and its characteristics. Free volume theories. Factors controlling T_g. Macromolecular dynamics in the amorphous state. The Rouse-Bueche theory. The de Gennes reptation theory. Different paths to a glass transition: cooling, compression, polymerization.</p> <p>The crystalline state in polymers. Evidences and characteristics of polymer crystal structures. Crystal structures for most common polymers. Characteristics of crystals obtained from either dilute solutions, melt cooling or solid-state polymerization. Polymer single crystals. Lamellae and spherulites. Semi-crystalline polymers and determination of the</p>
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	<p>degree of crystallinity. Crystal thickness. Oriented crystals and polymer fibres. Defects in polymer crystals. Kinetics and thermodynamics of crystallization.</p> <p>Melting of crystalline polymers. Equilibrium melting temperature. Factors that influence melting of polymers. Effects on the melting temperature of crystal thickness, chemical structure, molar mass, branching, copolymerization, annealing. Relationship between T_m and T_g. Differential scanning calorimetry (DSC): traditional power-compensation and heat-flux apparatuses, experimental procedures and calibration. Qualitative and quantitative interpretation of DSC thermograms. Modulated-temperature DSC (MTDSC), separation of reversing and non-reversing thermal events. Crystal perfection before melting.</p> <p>Elasticity of rubbers. Molecular structural requirements for a polymer to show elastomeric properties. Elastomers as entropic springs. Natural rubber. Vulcanization. Mechanical behaviour of elastomers. Thermodynamics of elastomer deformation. The thermoelastic inversion effects. Statistical theory of elastomer deformation. Effects of entanglements, loops and chain ends. Stress-strain behaviour of rubbers. Strain induced crystallization.</p> <p>Electrical properties of polymers. Survey on the variety of possible electrical properties within the class of polymeric materials. Brief review of the classical and the band models for current transport in conductors and semi-conductors. Inherently conducting polymers. Conjugated polymers and their molecular structure. The case of polyacetylene: structure, explanation of its conductivity, doping, polarons and solitons. Ionic conduction in polymers: electrophoresis of ionic species from ionomers or from impurities. Electrical properties of insulating matrix/conducting fillers composites. Percolative behaviour of the electrical conductivity. Factors influencing the critical value of the filler volume fraction. Polymers as insulators: the dielectric breakdown phenomenon and the dielectric strength of polymers. Polymer dielectrics: the different mechanisms of electric polarization occurring in polymers, behaviour under time varying electric fields, the complex dielectric permittivity and the dielectric spectrum. Dielectric relaxation processes and models for their description. Dielectric spectroscopy methods for measuring and analysing the complex permittivity spectrum. Dielectric spectrum of a glass former: recognizable patterns in the behaviour of dielectric constant and loss factor; multiple relaxations, dielectric parameters, ionic conduction. Discussion about the influence of temperature on the spectra and on the dielectric parameters of a supercooled glass former. Evolution of the dielectric spectra and of the dielectric parameters in time-varying systems: the case of polymerization reactions.</p>
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	<p>Dielectric analysis of chemically, thermally and mechanically induced glass transition: differences, analogies and attempts for a unified description of the glass transition. Microwave heating.</p> <p>Processing of polymers. Principles of the techniques for processing of polymers. low properties of polymer melts: bulk deformation, elongational flow (tension stiffening and tension thinning), shear flow (shear thinning). Melt flow index. Apparent viscosity as a function of temperature and molar mass. Viscoelasticity of molten polymers and swell ratio. Cooling and solidification of polymer melts. Extrusion. Injection moulding. Thermoforming. Blow moulding. Compression moulding. Transfer moulding.</p>
Examination	<p>The final exam is composed of a final oral examination which has a duration averaging between 40 and 60 minutes. During the oral exam the student can be also required to solve open questions/exercises/problems. The student will be assessed on his/her demonstrated ability to discuss the course contents with critical awareness and with property of expression by starting from problems/exercises/questions proposed by the exam commission. The oral test is not passed if the candidate demonstrates to not be able to express him/her-self in a clean and proper language and if the candidate does not correctly answer at least to those questions concerning the very basic parts of the course.</p>
Requirement for examination	
More information	CLASSIFICATION: MATERIALS SCIENCE
Learning outcomes	<p>The student who successfully completes the course:</p> <ul style="list-style-type: none"> - will be aware of the specific characteristics of the materials included into the class of polymers, particularly with respect to structure and properties; - will acquire knowledge of both mechanisms for synthesizing polymeric materials and relevant industrial production and processing technologies; - will acquire basic knowledge of the principal experimental techniques for characterizing physical-chemical properties of polymeric materials.

Course name	GREEN CHEMISTRY FOR MATERIALS AND PROCESSES		
Credit Points (ECTS) 6	Workload (Face-to Face) 48 hours	Duration 1 semester	Offered (Term) 1
Institution in charge	University of Pisa		
Instructors	Maurizia Seggiani		

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Purpose of the module	BIOPHAME Track	Mode
	All tracks	Optional
Contents	<p>The concepts that will be presented are the emerging ones of the Green Chemistry: atomic efficiency, heterogeneous catalysis and biocatalysis, replacement of solvents and toxic compounds, reaction and process intensification, conversion of biomass into valuable chemicals/materials, waste recycle, design and production of green products as bioplastics. Examples of industrial processes where this sustainability approach is adopted will be shown as extraction of active biomolecules and biopolymers from biomass with green solvents (supercritical fluids, ionic/eutectic liquids) and enzymatic technologies, modification of natural fibres with enzymes and green technologies (steam explosion, supercritical carbon dioxide, microwaves, etc).</p>	
Examination	Oral exam	
Requirement for examination	<p>Knowledge on the tools and methodologies for the assessment of chemical, toxicological and environmental risk, life cycle analysis of products and processes, environmental indicators, green design of chemicals, polymers, and materials.</p>	
More information	CLASSIFICATION: MATERIALS SCIENCE	
Learning outcomes	<p>After the completion of the course, the students will have the knowledge and skills useful in designing the construction of products, materials, and plants with minimal impact on human health and the environment.</p>	

Course name	COMPUTATIONAL MATERIALS SCIENCE		
Credit Points (ECTS) 6	Workload (Face-to Face) 48	Duration 1 semester	Offered (Term) 1
Institution in charge	University of Pisa		
Instructors	Giuseppe Brancato		
Purpose of the module	BIOPHAME Track	Mode	
	All tracks	Optional (recommended for Option A: Modelling & Simulation)	

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Contents	<p>Intermolecular Forces: Hydrogen bonding, Electrostatic interactions, London forces. Molecular clusters, Supramolecular assemblies.</p> <p>Thermodynamics: Variational formulation. Free energy of a reaction, Equilibrium constants.</p> <p>Statistical Mechanics: Gibbs ensemble, Mechanical system, Generalized coordinates, Lagrangian formalism. Hamiltonian formalism, Hamilton's equation, Phase space. Properties of Hamiltonian systems, Conservation laws, Canonical transformation, Poisson brackets, Liouville's operator, Equation of motion of a dynamical variables. Liouville's equation and theorem, Probability density, Microcanonical ensemble, Canonical ensemble.</p> <p>Molecular Dynamics: Definition, Foundations of molecular simulations, Limits and approximations. Overview of the basic ingredients (Energy potential, Force fields, Numerical integrators). Energy potential, Force fields, Numerical integrators. Force field terms (bonding, bending, torsion, non-covalent interactions). Molecular Dynamics: Coordinate and Velocity initialization, Integrators. Numerical integrators (velocity Verlet, Leapfrog), Statistical mechanical ensemble, Thermal and pressure coupling.</p> <p>Enhanced Sampling Methods. Simulation of the Kv ion channel.</p> <p>Simulation of a lipid bilayer.</p> <p>Fundamentals of enhanced sampling techniques. Implicit solvent and continuum electrostatic modeling. From collisional theory to stochastic dynamical systems. Stochastic differential equations and Statistical Mechanics. Structural properties: distribution functions, radial distribution functions.</p> <p>Monte Carlo methods: Numerical Integration, Importance sampling. Free Energy methods.</p> <p>Free Energy Methods: Thermodynamic Integration, Free energy perturbation, Umbrella Sampling</p> <p>Free Energy Methods: Metadynamics, Jarzinski method, Adiabatic free energy.</p>
Examination	Oral Exam. In addition to questions related to the basic knowledge of the course, students will be asked to present a scientific problem of their interest suitable to be treated with molecular modeling methodologies.
Requirement for examination	The aim of the course is to provide an overview of the theories and methodologies currently used in various fields of computational molecular sciences, ranging from biomedical sciences to material sciences. A special focus will be devoted to those models and algorithms related to molecular simulation techniques, including enhanced sampling and free energy methods. Such models will be illustrated along with relevant examples taken from recent literature and concerning different molecular modeling applications.
More information	CLASSIFICATION: PHYSICS-CHEMISTRY
Learning outcomes	On successful completion of the course students will be able to: - comprehend molecular modeling techniques currently used in the field of life and material sciences

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	<ul style="list-style-type: none"> - develop competences on some of the most common computational methodologies used in molecular sciences - develop computational skills through tutorials and exercises
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Course name	SPECTROSCOPY of NANOMATERIALS - 1		
Credit Points (ECTS) 6	Workload (Face-to Face) 36 hours	Duration 1 semester	Offered (Term) 1
Institution in charge	University of Pisa		
Instructors	Alessandra Toncelli		
Purpose of the module	BIOPHAME Track	Mode	
	All tracks	optional	
Contents	<p>Basics of radiation/matter interaction and understanding of emission/absorption spectra of substances in the range near-UV - IR, up to the THz range.</p> <p>Technical and conceptual tools for emission, absorption, Raman spectroscopy.</p> <p>Energy levels of the main physical systems: electronic levels in atoms and molecules, rotational and vibrational levels of molecules, Lorents-Drude model, electronic levels of impurities (transition metals and rare earths) in crystals, electronic and fononic bands in crystals.</p> <p>Group theory applied to the main energy level systems mentioned above.</p>		
Examination	Oral final exam, partly fulfilled through a short presentation on a topic chosen agreement with the lecturers.		
Requirement for examination			
More information	CLASSIFICATION: PHYSICS		
Learning outcomes	<p>On successful completion of the course students will gain the ability to analyze problems of optics involving nanomaterials, both for the analysis at the local scale and for the exploitation of their specific properties in devices and approaches.</p> <p>Although the major emphasis is put onto the physical aspects, the course fosters the development of cross-disciplinary abilities, directly connected with other scientific areas.</p>		

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Course name	RHEOLOGY		
Credit Points (ECTS) 6	Workload (Face-to Face) 48 hours	Duration 1 semester	Offered (Term) 1
Institution in charge	University of Pisa		
Instructors	Laura Andreozzi		
Purpose of the module	BIOPHAME Track	Mode	
	All tracks	optional	
Contents	<p>1) The viscosity of liquids: introduction to rheology</p> <p>2) Flow and deformation: introduction; shear rate and shear stress; dimensions and units</p> <p>3) The newtonian liquid: viscosity; variation of viscosity with temperature; effects of pressure; limit of newtonian behaviour</p> <p>4) Some equations for the flow of newtonian liquid: flow in rotational viscometer; flow in straight circular pipes; spheres falling in newtonian liquids; other important flows</p> <p>5) Viscometry: some important things about using viscometers; viscometer design.</p> <p>6) Shear—thinning liquid: qualitative features of flow curves; mathematical description of flow curves: models</p> <p>7) Equations for the flow of non – newtonian fluids: some selected examples</p> <p>8) Yield stress fluids: history of the yield stress and yield stress values; flow equations with yield stress</p> <p>9) The flow of “solids”: non-linear “viscosity” of solids</p> <p>10) Linear viscoelasticity and time effects: introduction; mechanical analogues of viscoelastic behavior; measuring linear viscoelasticity : creep and oscillatory tests, response of model materials and real systems; relationship between oscillatory and steady-state viscoelastic parameters; stress relaxation testing and start-up experiments.</p> <p>11) Non- linear viscoelasticity: everyday elastic liquids; some visible viscoelastic manifestations; proper description of viscoelastic forces and their measurements; some viscoelastic formulas</p> <p>15) The flow of suspensions: viscosity of dispersions and emulsions; effects of the shape and size of the particles; overview of particle interactions; viscosity of flocculated systems; thixotropy; shear thickening</p> <p>16) Polymer rheology: different kinds of polymer chains; polymer solutions; polymer melts</p> <p>17) Rheology of surfactant systems: surfactant phases; rheology of surfactant systems</p> <p>18) Rheology of food products</p> <p>19) Extensional flow: the extensional flow; the Trouton ratio; examples of extensional viscosity curves; some applications</p> <p>20) Recall on scalars, vectors, tensors and their algebra.</p>		

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	<p>21) The stress tensor . Construction, property.</p> <p>22) Stress ellipsoid. The case of pressure . Deformation tensor.</p> <p>23) Generalized Hooke's law. Matrix of modules and compliance , its properties. Recalls: differential operators on scalars / vectors / tensors, useful theorems.</p> <p>24) Conservation of the moment and the mass. Newtonian constitutive equations. Navier Stokes equation. Problems on the flow of incompressible Newtonian fluids: entrainment, f. of poiseuille, f. torsional</p> <p>25) Material functions and experimental response to steady state flow in simple shear geometry and in extensional geometry.</p> <p>26) Viscoelasticity and constitutive equations</p> <p>27) Non-linear viscoelasticity. Cauchy and Finger Tensors.</p> <p>28) Introduction to more advanced constitutive equations. Models: Integral Lodge, Maxwell Upper / Lower Convected, Cauchy-Maxwell, Rubberlike Liquid Lodge. Quasi-linear models (fluid A and B), non-linear differentials (Oldroyd 8 const.)</p> <p>29) Other constitutive approaches: molecular approach for polymeric systems. Outline: Configuration distribution function, temporary network model, reptation theory</p>
Examination	The modality of verification of the students knowledge and skills foresees the continuous interaction with the teacher during the lessons as well as a final oral exam and a presentation of a seminar on a topic previously agreed with the teacher
Requirement for examination	
More information	CLASSIFICATION: PHYSICS
Learning outcomes	<p>On successful completion of the course students will be able to:</p> <ul style="list-style-type: none"> - Be aware of the importance of rheology in scientific research, in industrial applications and in life, including daily activities; - know the main rheological behaviors of the materials; - recognize the rheological behavior of different materials; - apply the main rheological models; - know the experimental methods of rheological survey and main instrumentation; - know the mathematical tensor treatment of rheology..

Course name	Biofluids and Materials Interactions		
Credit Points (ECTS) 3	Workload (Face-to Face) 24 hours	Duration 1 semester	Offered (Term) 1
Institution in charge	University of Pisa		
Instructors	Serena Danti		

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Purpose of the module	BIOPHAME Track	Mode
	All tracks	compulsory
Contents	<p>Introduction to biofluid mechanics: Definitions of fluid, fluid hydrostatics and fluid dynamics; pressure and shear stress; fluid properties (density, viscosity); types of fluids (Newtonian, non-Newtonian); types of fluid flow (laminar, turbulent).</p> <p>Fluids in the human body, Blood-material interactions: Blood fluid dynamics; the influence of materials surface.</p> <p>Fluid materials interacting with gas and sound waves. Metal corrosion in biofluids.</p>	
Examination	Oral Exam	
Requirement for examination		
More information	CLASSIFICATION: CHEMISTRY	
Learning outcomes	<p>On successful completion of the course students will be able to:</p> <ul style="list-style-type: none"> - Know the biofluid mechanics - know the basics of biofluid in human body - know the interactions of fluids with gas and sound waves 	

Course name	SURFACE SCIENCE		
Credit Points (ECTS) 3	<p>Workload (Face-to Face)</p> <p>The course is composed by 24 hours: at least 18 hours of class teaching and one visit to research laboratories where experiments of surface physics using scanning probe microscopy are performed</p>	Duration 1 semester	Offered (Term) 1
Institution in charge	University of Pisa		
Instructors	Massimiliano Labardi		
Purpose of the module	BIOPHAME Track	Mode	

BIOPHAM Master - Syllabus of the courses proposed at the University of Pisa (UNIFI)

	All tracks	Optional
Contents	<p>PART I: Phenomenology of surfaces and interfaces</p> <p>Introduction to the course. Introduction to surfaces and interfaces. Surface/volume ratio. Microscopic interpretation of intermolecular forces. Interaction energy between ions, frozen and mobile permanent dipoles. Keesom energy.</p> <p>Interaction energy with induced dipoles: Debye induction energy, London dispersive energy. Frequency dependence of atomic polarizability. Ionization energy. Van der Waals energy.</p> <p>Additivity of Van der Waals interaction. VdW forces between macroscopic bodies: adsorption, adhesion, cohesion. Hamaker constant. Liquid surfaces. Interfacial thickness. Surface free energy and surface energy. Surface tension. Thermodynamics of interfaces in equilibrium: Gibbs theory. Definition of interface and Gibbs dividing plane. Interfacial excess.</p> <p>Thermodynamic potentials at the interface. Thermodynamic definition of surface tension. Euler relation and Gibbs-Duhem relation. Surface tension and interfacial excess. Mixing entropy and mixing chemical potential. Surface activity: case of ionic, apolar, and amphiphilic solutes. Colloidal aggregates. Critical micellar concentration. Thermodynamics of colloidal aggregation.</p> <p>Pressure difference across a curved surface: Young-Laplace equation. Vapor pressure at a curved surface: Kelvin equation. Supersaturation pressure. Theory of homogeneous nucleation. Heterogeneous nucleation. Wetting. Wetting line and contact angle. Young equation. Cases of partial, complete, and no wetting. Capillarity phenomena. Thin film formation. Dewetting. Pseudo partial wetting and wetting layer. Thin film deposition: dip coating and spin coating.</p> <p>PART II: Surface characterization techniques</p> <p>Scanning probe microscopy. Beam vs local probes. Atomic force microscope. Working principle: typical setup. Piezoelectric scanners and raster scan. Constant height mode and constant force mode. Interaction steepness and atomic resolution. Cantilever force sensors. Optical lever deflection detection method. Static mode of operation: contact mode. Jump-in-contact and jump-off-contact points. Lateral force and local friction coefficient measurement. Bidirectional optical lever.</p> <p>Dynamic modes of AFM. Problems arising in static mode: thermal noise. Response function of the cantilever as a simple harmonic oscillator. Tapping mode. Phase sensitive coherent detection and lock-in detection. Effect of conservative and dissipative interactions on resonance curve. Frequency-modulation mode. Piezoelectric resonant force sensors: quartz tuning fork.</p> <p>Combined scanning probes. Auxiliary distance control. Electrostatic Force Microscopy. Dependence of electric force on distance and electric properties of dielectrics. Voltage-modulated force detection. Dielectric constant, surface charge and contact potential measurement. Kelvin probe method. Kelvin probe force microscopy.</p> <p>Nanotribology. Friction at a contact point measured by AFM. Stick-slip model for dissipation by dynamical friction. Friction of atomic layers.</p>	

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	Quartz crystal microbalance (QCM). Gravimetric and non-gravimetric QCM. Interfacial viscosity and slip time.
Examination	Oral exam, or presentation, in seminar form, of a detailed study concerning one of the topics of the course.
Requirement for examination	
More information	CLASSIFICATION: PHYSICS
Learning outcomes	On successful completion of the course students will be able to be introduced to the physics of surfaces and interfaces, focusing on basic concepts rather than specific details, and to be able to know the physical phenomena underlying some of the most important techniques and methods for surface analysis.