**BIOPHAM Master - Syllabus of the courses proposed in**
**Track 1: Pharmaceutical Materials Science (ULille-UPC-ULille)**

| TERM 1 – University of Lille (ULille) – France | | | | |
|---|---|---|---|---|
| **Course name** | **Classification** | **ECTS** | **Hours face-to-face in class** | **Compulsory/optional Recommendation** |
| Continuum mechanics | Physics | 3 | 24h | Compulsory |
| Introduction to Pharmaceutical Materials Science | Materials Science | 6 | 48h | Compulsory |
| Drug product development and pharmaceutical technology I | Pharmacy | 3 | 24h | Compulsory |
| AI and advanced computational methods in physics | Physics | 3 | 25h | Compulsory |
| Atomic scale modeling I – Classical methods | Physics | 3 | 28h | Compulsory |
| States of Matter and Materials Science Primers | Materials Science | 3 | 24h | Compulsory |
| Tutored trainings | Physics | 3 | 10.5h | Compulsory |
| Course from the Graduate Program | N/A | 3 | 20h | Compulsory |
| Foreign language (French or English) | N/A | 3 | 24h | Compulsory |
| **TOTAL** | | **30** | **227h** | |

<table>
<tr><th colspan="4">TERM 1 – University of Lille (ULille) – France</th></tr>
<tr><td>Course name</td><td colspan="3">Continuum mechanics</td></tr>
<tr><td>Credit Points (ECTS) 3</td><td>Hours (Face-to Face in class):<br>Lectures: 24h<br>Practical works: -<br>Total: 24h</td><td>Duration<br>1 semester</td><td>Mode<br>Compulsory</td></tr>
<tr><td>Instructors</td><td colspan="3">Philippe Carrez (Resp.), Patrick Cordier, Sébastien Merkel</td></tr>
<tr><td>Contents</td><td colspan="3">Continuum mechanics is a fundamental theory of many fields of science and engineering. This course will give an introduction to the principles of stress, strain, anisotropic and isotropic elasticity with applications covering a broad area relating to the mechanical behavior of materials.<br>Objectives:<br>• Acquire the basic concepts of continuum mechanics<br>• Define and manipulate stress and strain tensor, apply tensor transformation<br>• Analytically solve simple problems of elasticity<br>Course outline:<br>• Stress and strain as a second-rank tensor<br>• Fondamental equations of elasticity, Hooke’s law<br>• Navier equations<br>• Review of macroscopic plastic behavior of matter<br>• Principles stresses and yield criterion</td></tr>
<tr><td>Skills acquired</td><td colspan="3">Students will be able to manipulate fundamental equations of elasticity theory and acquire knowledge of several techniques of resolution of different problems at different length scales.</td></tr>
<tr><td>Examination</td><td colspan="3">Written final exam</td></tr>
<tr><td>Classification</td><td colspan="3">Physics</td></tr>
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**Track 1: Pharmaceutical Materials Science (ULille-UPC-ULille)**

<table>
<tr><th colspan="4">TERM 1 – University of Lille (ULille) – France</th></tr>
<tr><td>Course name</td><td colspan="3">Introduction to Pharmaceutical Materials Science</td></tr>
<tr><td>Credit Points (ECTS) 6</td><td>Hours (Face-to Face in class):<br>Lectures: 44h<br>Practical works: 4h<br>Total: 48h</td><td>Duration<br>1 semester</td><td>Mode<br>Compulsory</td></tr>
<tr><td>Instructors</td><td colspan="3">Emeline Dudognon (Resp.), Natalia Correia, Frédéric Affouard</td></tr>
<tr><td>Contents</td><td colspan="3">The course provides an introduction to pharmaceutical materials science by presenting molecules, their interactions, and the nature of ordered and disordered associated materials and their transformations. It also introduces key experimental methods for structural and thermodynamic characterization.<br>The objective of this course is to provide students with in-depth exploration of pharmaceutical materials, focusing on three main aspects: i) The basic components of materials—atoms, molecules, and ions—and their associated interactions; ii) The structural description of materials, ranging from disordered to ordered states, along with experimental techniques such as X-ray diffraction; iii) The thermodynamics and state transformations of materials, as well as thermal analysis techniques.<br>i) Basic elements and interactions.<br>Atoms, ions, molecules. Concepts of isomerism and conformations. Chirality. Functional groups in molecules. Study of some simple functions: alkanes, alkenes, alkynes, aromatic hydrocarbons, alcohols, amines, etc. Intermolecular interaction (ionic forces, hydrogen bonding, van der Waals interactions) and intermolecular interactions (metallic, ionic and covalent bond). Major classes of molecules and specificities (carbohydrates, polymers, biopolymers…)<br>ii) Structure<br>The perfect crystal (reminders), space group, relationship to X-ray diffraction. Thermal agitation. Vacancies. Alloys. Statistical description of monatomic fluids and amorphous materials, order-disorder transitions. Semi-ordered states: solutions, colloidal systems, polymers, mesomorphic phases. Size effects and nanostructures: experimental identification. Nanostructural organizations: short- and medium-range order in amorphous materials.<br>iii) Thermodynamics<br>Fundamentals of thermodynamics of molecular materials in the crystalline/amorphous forms and transformation of states. Thermodynamics and phase diagrams - Thermodynamic classification of phase transitions - Stability, metastability and instability - Physical states: crystalline polymorphs, mesophases, amorphous. Introduction to thermodynamics of multicomponent systems: Construction and interpretation of binary phase diagrams. Gibbs free energy diagrams as a function of mixture composition. Binodal & spinodal. Precipitations. Eutectic systems. Miscibility, and solubility. Introduction to calorimetric and thermal techniques (TGA/DSC): Definitions, interpretation of curves, usefulness of techniques for the construction of phase diagrams.<br><br>The lectures are complemented by a 4-hour lab practical session on Differential Scanning Calorimetry (DSC) and X-ray diffraction techniques, focusing on the</td></tr>
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| | exploration of physical states (crystalline vs. amorphous) and their transformations, including melting, crystallization, and vitrification. |
| Skills acquired | On successful completion of the course, students will be able to:<br>• Know the basic elements (atoms, ions, molecules) of materials and their interactions.<br>Have general knowledge of the structure and microstructure of different states of matter.<br>• Have a basic understanding of the main structural and thermodynamical experimental characterization methods.<br>• Understand and analyse scientific reports concerning experimental studies concerning structure and thermodynamics of ordered and disordered condensed matter systems |
| Examination | 1 final written exam<br>1 report based on the practical session<br>1 oral presentation |
| Classification | Materials Science |

<table>
<tr><th colspan="4">TERM 1 – University of Lille (ULille) – France</th></tr>
<tr><td>Course name</td><td colspan="3">Drug product development and pharmaceutical technology I</td></tr>
<tr><td>Credit Points (ECTS) 3</td><td>Hours (Face-to Face in class):<br>Lectures: 16h<br>Practical works: 8h<br>Total: 24h</td><td>Duration<br>1 semester</td><td>Mode<br>Compulsory</td></tr>
<tr><td>Instructors</td><td colspan="3">Juergen Siepmann (Resp.), Florence Siepmann, Mounira Hamoudi, Youness Karrout, Susanne Florin Muschert</td></tr>
<tr><td>Contents</td><td colspan="3">This course provides hands-on and theoretical training in drug formulation, manufacturing, and quality control of various pharmaceutical dosage forms. It emphasizes regulatory compliance, excipient selection, and practical techniques for ensuring product quality and performance.<br>This course introduces students to drug product development and pharmaceutical technology, covering formulation, manufacturing, and quality control of key dosage forms. It explores tablets, capsules, creams, implants, and more, along with the role of APIs and excipients. Students learn to evaluate dosage form advantages, select appropriate excipients, and apply regulatory standards. Practical training includes preparation techniques like granulation and film coating, and quality tests such as dissolution and disintegration. Emphasis is placed on hands-on use of equipment, handling formulation challenges, and ensuring product quality.<br>This course will provide an introduction to drug product development and Pharmaceutical Technology. The students will obtain an overview on the formulation, manufacturing and quality control strategies of the most important pharmaceutical dosage forms administered via different routes, e.g. orally, topically or via injection/implantation. This will include tablets, capsules, pellets, ointments, creams, microparticles and implants. The importance of the key properties of the active pharmaceutical ingredients (APIs) and commonly used excipients (inactive ingredients) will be treated. Students will get familiar with the advantages and disadvantages of the different pharmaceutical dosage forms. They will learn how to choose the most appropriate types of excipients and manufacturing processes. The course will also provide an introduction into the key characterization methods requested by the regulatory authorities to control the quality of the drug products, according to the European and United States Pharmacopeia.<br>This course will also provide practical training on different preparation techniques for drug products (e.g., wet granulation, compression, film coating) and the most important characterization techniques described in the European and United States Pharmacopoeia (e.g., drug dissolution testing, disintegration measurements). The students will gain a thorough understanding of specific apparatuses which can be used to manufacture drug products and control their quality. They learn how to handle drugs and a variety of excipients (e.g. for direct compression or wet granulation). They will get used to measure tablet hardness, friability, tab density, particles sizes and powder flow behavior. The students will get familiar with different types of equipment and quality control tests, including those suitable for the manufacturing and characterization of time-controlled</td></tr>
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| | drug delivery systems and drug products containing poorly water-soluble drugs. Special emphasis will be placed on common practical pitfalls and challenges. |
| Skills acquired | On successful completion of the course students will:<br>• Have knowledge of the how a drug substance can be administered to a patient<br>• Be familiar with the most important pharmaceutical dosage forms (e.g. tablets, capsules, pellets, ointments, creams).<br>• Have knowledge of pharmaceutical materials, in particular excipients and their specificities<br>• Know the main approaches used for the manufacturing and quality control of drug products<br>• Differentiate the various preparation methods for drug products, their practical advantages and disadvantages<br>• Know the most adapted experimental techniques to prepare drug products<br>• Apply the key characterization methods for a variety of pharmaceutical dosage forms<br>• Be familiar with the common pitfalls and challenges related to state-of-the-art manufacturing equipment for pharmaceutical products |
| Examination | 1 final oral exam<br>1 report based on the lab practical session |
| Classification | Pharmacy<br>The classes will be held at the College of Pharmacy (University of Lille). |

| **TERM 1 – University of Lille (ULille) – France** | | | |
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| Course name | AI and advanced computational methods in physics | | |
| Credit Points (ECTS) 3 | Hours (Face-to Face in class):<br>Lectures: 15h<br>Practical works: 10h<br>Total: 25h | Duration<br>1 semester | Mode<br>Compulsory |
| Instructors | Quentin Coopman (Resp.), Jérôme Riedi | | |
| Contents | Explore the intersection of AI, Machine Learning, and Physics in this class. Gain hands-on experience with cutting-edge techniques and applications tailored for the world of physics.<br>Objectives :<br>This class introduces AI and Machine Learning, focusing on their applications in physics. It covers fundamental concepts like supervised and unsupervised learning, regression, and classification, as well as advanced topics such as neural networks and deep learning. Students will explore classification techniques, clustering algorithms, and data preprocessing methods tailored for physics data. The course also delves into dimensionality reduction and advanced subjects like physics-informed machine learning. By the end, students will be equipped to apply AI and ML techniques effectively in the field of physics.<br>Courses (10H):<br>I - Introduction to Artificial Intelligence and Machine Learning (1H)<br>Overview of AI and ML, Applications in physics, Key concepts and terminology<br>II - Fundamentals of Machine Learning (1H)<br>Supervised vs. unsupervised learning, Regression, classification, prediction<br>Evaluation metrics<br>III - Classification/Clustering algorithms (1H30)<br>Linear Models and Regularization (Linear regression), Decision Trees and Ensemble Methods (Decision trees, Random, Gradient boosting regression tree forests), K-means<br>IV - Dimensionality reduction (e.g., Principal Component Analysis) (45 mins)<br>V - Neural Networks and Deep Learning (2H15)<br>Introduction to neural networks, Activation functions, Training neural networks<br>Encodeur/Decodeur<br>VI - Data Preprocessing (1H)<br>Handling physics data, Feature selection and extraction, Data normalization and scaling, Datacentric methods<br>VII - Introduction Advanced Topics in Machine Learning for Physics (2H)<br>Physics-informed machine learning, Interpretable AI models<br><br>Practicals (15H):<br>The practical sessions will cover the themes discussed in the lecture courses, namely: Linear models (3H), K-means (2H), Principal Component Analysis (2H), Neural Networks (3H), Deep Learning (3H), Data Preprocessing (2H) | | |
| Skills acquired | Skills acquired | | |

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| | • Grasp the fundamental principles of artificial intelligence and machine learning.<br>• Learn key terminology and concepts used in AI and ML.<br>• Apply AI and ML techniques to solve problems in the field of physics.<br>• Differentiate between and apply supervised and unsupervised learning techniques.<br>• Implement regression, classification, and prediction models.<br>• Use popular ML libraries and tools such as TensorFlow, PyTorch, and scikit-learn.<br>• Implement AI and ML techniques in practical, hands-on projects and case studies.<br>• Use advanced digital tools autonomously for one or more professions or research sectors in the field.<br>• Conduct a reflective and distanced analysis, considering the issues, challenges, and complexity of a request or situation, to propose appropriate and/or innovative solutions in compliance with regulatory developments.<br>• Develop predictive tools based on validated models describing complex physical problems.<br>• Program digital tools to process physical measurements in a relevant manner (potentially using machine learning and AI approaches). |
| Examination | Continuous assessment and project<br>The course evaluation will consist of two main parts:<br>• Multiple Choice Quiz at the beginning of some lectures (30%)<br>• Project leading to a written report of analysis and interpretation of a dataset (70%) |
| Classification | Physics |

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<tr><th colspan="4">TERM 1 – University of Lille (ULille) – France</th></tr>
<tr><td>Course name</td><td colspan="3">Atomic scale modeling I – Classical methods</td></tr>
<tr><td>Credit Points (ECTS) 3</td><td>Hours (Face-to Face in class):<br>Lectures: 12h<br>Practical works: 16h<br>Total: 28h</td><td>Duration<br>1 semester</td><td>Mode<br>Compulsory</td></tr>
<tr><td>Instructors</td><td colspan="3">Céline Toubin (Resp.), Frederic Affouard, Charlotte Bequart, Philippe Carrez</td></tr>
<tr><td>Contents</td><td colspan="3">Discover powerful simulation techniques like Molecular Dynamics and Monte Carlo to predict and design material properties at the atomic scale.<br><br>Objectives:<br>• Identify when and why to use atomistic simulations in research and development.<br>• Apply optimization techniques to obtain stable atomic or molecular structures.<br>• Set up and adapt force-field models for different material systems.<br>• Get the principles of Monte Carlo methods for configurational sampling.<br>• Analyze simulation outputs using relevant physical and statistical quantities.<br><br>Course outline<br>• Why performing simulations?<br>• Optimization Techniques<br>• Force-field description<br>• Molecular dynamics principles: forces evaluation and cut off, periodic boundary conditions, minimum image convention, thermostat, barostat, statistical averages and observables<br>• Monte Carlo<br>• Hands on practicals</td></tr>
<tr><td>Skills acquired</td><td colspan="3">• Optimize atomic structures using energy minimization and relaxation techniques.<br>• Identify appropriate simulation methods (MD or MC) for solving material and molecular-scale problems.<br>• Understand and evaluate force-field models for specific systems to achieve reliable predictive accuracy.<br>• Implement key MD concepts, including thermostats, barostats, cutoffs, and periodic boundary conditions.<br>• Apply statistical mechanics principles to extract thermodynamic and structural observables from simulation data.</td></tr>
<tr><td>Examination</td><td colspan="3">Report<br>Oral presentation</td></tr>
<tr><td>Classification</td><td colspan="3">Physics</td></tr>
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<tr><th colspan="4">TERM 1 – University of Lille (ULille) – France</th></tr>
<tr><td>Course name</td><td colspan="3">States of Matter and Materials Science Primers</td></tr>
<tr><td>Credit Points (ECTS) 3</td><td>Hours (Face-to Face in class):<br>Lectures: 24h<br>Practical works: -<br>Total: 24h</td><td>Duration<br>1 semester</td><td>Mode<br>Compulsory</td></tr>
<tr><td>Instructors</td><td colspan="3">Valérie Gaucher (Resp.), Tiana Deplancke, Sophie Barrau, Franck Beclin, Mathieu Touzin</td></tr>
<tr><td>Contents</td><td colspan="3">Objectives:<br>This course aims to present the different classes of materials based on their chemical bonds. The microstructure and the specific properties Three major classes of materials will be detailed: ceramics, metal and alloys and polymers.<br>Outline:<br>• Generalities: the state of matter, crystalline and amorphous materials, Phenomenological approach of the diffusion process in gas and solid.<br>• Introduction to material science: Chemical bounding and the resulting physical and mechanical properties. Ashby diagram and main classes of materials.<br>• Ceramics: Introduction, properties and applications, diffusion process and elaboration process (sintering ...)<br>• Metals and alloys: Definition and structure, Phase diagram, phase transformation and microstructure resulting. Study case: Steel and iron carbon diagram.<br>• Polymers: Definition, macromolecular conformation, viscosity, classification of polymers, phenomenological and thermodynamical approaches of the glass transition, nucleation and growth of crystals, melting behavior.</td></tr>
<tr><td>Skills acquired</td><td colspan="3">By the end of this course, students will have a clear understanding of the different families of materials (metals and alloys, polymers, ceramics). They will know the main characteristics (structure, end use properties).</td></tr>
<tr><td>Examination</td><td colspan="3">Written exam</td></tr>
<tr><td>Classification</td><td colspan="3">Materials science</td></tr>
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<tr><th colspan="4">TERM 1 – University of Lille (ULille) – France</th></tr>
<tr><td>Course name</td><td colspan="3">Tutored trainings</td></tr>
<tr><td>Credit Points<br>(ECTS) 3</td><td>Hours (Face-to Face in class):<br>Lectures: 10.5h<br>Practical works: -<br>Total: 10.5h</td><td>Duration<br>1 semester</td><td>Mode<br>Compulsory</td></tr>
<tr><td>Instructors</td><td colspan="3">Sébastien Merkel</td></tr>
<tr><td>Contents</td><td colspan="3">Discovery of new topics in physics based on the scientific literature and develop your teaching and presentation skills in front of your peers.<br><br>Objectives<br>Promote scientific openness among Physics Masters students. Complement their training in subjects not covered in traditional courses. Develop students' ability to work independently using information from the literature. Develop professional skills (oral presentation, scientific writing, and poster presentation<br><br>Course outline<br>Students choose 1 work topic in pairs. Topics are proposed by department staff, based on scientific articles, books, etc and can cover any field of physics. The teaching consists in 6 in-person session guided by a main instructor, assistance from tutors, and significant personal work from the students based on information found in the University library and the scientific literature.<br>In person activities:<br>• Class 1 (1h30 CTD) Introduction, choice of subject, expectations<br>• Class 2 (1h30 TD, 3 groups): Mid-course presentation, 10 minutes per pair, plan<br>• Class 3 (1h30 TD, 3 groups) Presentation analysis session (based on students reports on the presentations of others, and on their own)<br>• Class 4 (1h30 CTD) Latex and overleaf<br>• Class 5 (1h30 CTD) Report preparation<br>• Class 6 (1h30 TD, 3 groups) Final oral<br>Tutor activities:<br>• propose a lead for topic (title, keywords, and references)<br>• 3 individual meetings with the student pair they supervise<br>➢ First contacts, first publications<br>➢ Assessment of students' individual research and understanding of the topic<br>➢ Detailed plan of report<br>• Proofreading and evaluation of reports<br>• Participation in evaluation of oral defenses</td></tr>
<tr><td>Skills acquired</td><td colspan="3">Develop advanced and critical expertise at the edge of knowledge in a sub-field of physics based on documents from the recent scientific literature<br>Identify, select, and critically analyze specialized resources to document a topic and make a synthesis and exploit their content<br>Present advanced scientific content in front of your peers</td></tr>
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| Examination | Report<br>Oral presentation |
| Classification | Physics, Materials science |

| **TERM 2 – Polytechnic University of Catalonia (UPC) – Spain** | | | | |
|---|---|---|---|---|
| **Course name** | **Classification** | **ECTS** | **Hours face-to-face in class** | **Compulsory/optional Recommendation** |
| Molecular and soft condensed matter | Physics-Chemistry | 4 | 36 | Compulsory |
| Materials science of drugs | Materials Science | 4 | 36 | Compulsory |
| Large facilities: synchrotron and neutron sources | Materials Science | 5 | 45 | Compulsory |
| Stochastic methods for optimization and simulation | Physics | 4 | 36 | Compulsory |
| Biopham Short Internship | Depends on the project | 5 | 45 | Compulsory |
| Complexity in biological systems | Biophysics | 4 | 36 | Optional 2 courses to be chosen out of 3 |
| Biophysical and materials science characterisation | Physics-Chemistry | 4 | 36 | |
| Machine learning with neural networks | Physics | 4 | 36 | |
| **TOTAL** | | **30** | **270** | |

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<tr><th colspan="4">TERM 2 – Polytechnic University of Catalonia (UPC) – Spain</th></tr>
<tr><td>Course name</td><td colspan="3">Materials science of drugs</td></tr>
<tr><td>Credit Points (ECTS) 3</td><td>Hours (Face-to Face in class):<br>Lectures: 30<br>Practical works: 6<br>Total: 36</td><td>Duration:<br>half semester</td><td>Mode<br>Compulsory (Tracks 1 and 2)</td></tr>
<tr><td>Instructors</td><td colspan="3">J. Ll. Tamarit, P. Lloveras, M. Romanini</td></tr>
<tr><td>Contents</td><td colspan="3">1. Basics concepts of crystallography<br>Translational order, unit cell, Bravais lattices. Point groups, space groups, crystal systems. Crystallographic planes, reciprocal lattice, Miller indices. From crystal system to molecular structure and geometry: crystals with a base and molecular crystals. Calculation and modelling of diffraction patterns from atomic and structure scattering factors. Solid-state polymorphism of drugs and other organic molecules.<br>2. Phase Equilibrium and phase transitions<br>Thermodynamic Potentials for hydrostatic pvT systems; Maxwell relations; TdS equations; General conditions for equilibrium; Fluctuations; Le Châtelier principle.<br>3. Phase transitions and topological pressure-temperature phase diagram<br>Equilibrium conditions for hydrostatic pvT systems; First-order phase transitions: Clausius-Clapeyron equation. Stability and metastability domains; High-order phase transitions. Group-subgroup phase transitions.; Critical and triple points; Topological P-T phase diagram. Calorimetry techniques.<br>4. Binary systems<br>Thermodynamics of mixing, thermodynamic potential; types of binary phase diagrams: eutectic, metatectic and peritectic; solubility and miscibility; metastable and unstable states; nucleation vs spinoidal decomposition.</td></tr>
<tr><td>Skills acquired</td><td colspan="3">On successful completion of the course, the students will be able to discuss the crystallographic properties of different polymorphs, the equilibrium conditions for a phase or phase coexistence, draw multiphase and/or binary phase diagrams, and distinguish between different equilibrium, metastable, and unstable states, and their relevance for drug formulations.<br>Students will learn to distinguish and characterize the different structural phases based on their symmetries and the relationships between them. The student will be able to apply concepts related to the thermodynamics of binary systems.</td></tr>
<tr><td>Examination</td><td colspan="3">Written exam, laboratory reports<br>Final Exam: 80%<br>Laboratory reports 20%</td></tr>
<tr><td>Classification</td><td colspan="3">Materials Science</td></tr>
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<tr><td colspan="4">TERM 2 – Polytechnic University of Catalonia (UPC) – Spain</td></tr>
<tr><td>Course name</td><td colspan="3">Molecular and soft condensed matter</td></tr>
<tr><td>Credit Points (ECTS) 3</td><td>Hours (Face-to Face in class):<br>Lectures: 36<br>Practical works: 0<br>Total: 36</td><td>Duration<br>half semester</td><td>Mode<br>Compulsory (Tracks 1 and 2)</td></tr>
<tr><td>Instructors</td><td colspan="3">R. Macovez, C. Alemán, M. Romanini</td></tr>
<tr><td>Contents</td><td colspan="3">(1) Basics of molecular condensed matter<br>1.1) Introduction on disorder & dynamics (liquids, mesophases, polymers, glasses); microscopic constituents, degrees of freedom, dynamics & disorder<br>1.2) statistical physics: entropy, Boltzmann statistics; partition function, energy, free energy<br>1.3) Mechanical & (di)electric properties: Eyring model & viscosity; elasticity & viscoelasticity; charge conduction & polarization; linear response theory in the time & frequency domains<br>1.4) Phase transitions, melting & crystallization, Avrami law; glass transition<br>1.5) Statistical models in soft matter: inter-particle interactions; hard-sphere gas, liquid & glass<br>(2) Single-component systems<br>- Structural glasses, residual entropy; Adam-Gibbs theory; relaxation & ageing<br>- Orientationally disordered solids, plastic crystals, Condis crystals<br>- Thermotropic liquid crystals: order parameter, Maier-Saupe theory, anisotropic properties<br>- Amorphous & semicrystalline linear polymers; Miller theory; rotational isomeric state model; Kuhn ideal chains; Rouse model, normal & segmental relaxations; viscoelasticity; reptation<br>- Polymers networks & rubber elasticity; conductive polymers; liquid crystal polymers; fibers<br>(3) Binary and multicomponent systems<br>- Binary systems: free energy of mixing, equilibrium phase diagrams; glass-forming mixtures<br>- Binary polymer systems: polymer blends; polymer solutions and gels; swelling phenomena; Flory-Huggins theory; block copolymers; water-surfactant mixtures, lyotropic liquid crystals<br>- Hydrogels, organogels, swelling phenomena; superhydrophobic/hydrophilic, superolephobic, superamphiphilic, and self-healing polymer coatings<br>- Self-assembly in condensed matter: biopolymers, helix-coil & coil-globule transitions; surfactant systems, biomembranes, emulsions; semiflexible polymers & cytoskeleton<br>- Applications to drug encapsulation, controlled drug release, and drug delivery</td></tr>
<tr><td>Skills acquired</td><td colspan="3">At the end of the course, students should be able to:<br>- based on the shape and size of its microscopic constituents, describe the types of condensed phases that can be displayed by a single-component systems, and ascertain which of them are observed at lower or higher</td></tr>
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| | temperature;<br>- describe the main experimental techniques available to identify phases and study molecular dynamics and phase transitions, and explain linear response theory and its main implications<br>- discuss the degree of disorder inherent to a condensed phase, and its main characteristic microscopic dynamic processes; discuss the role of disorder and molecular and macromolecular dynamics for rheological and mechanical properties<br>- describe orientational order in liquid crystals, and the resulting anosoptropy of mechanical, dielectric and optical properties<br>- use random walk models, self-similarity, entropic elasticity models and affine deformation theory to explain the properties of linear polymers, entangles polymer melts, and of polymer networks such as rubbers<br>- describe the phenomenology of the glass transition in a number of systems ranging from atomic and molecular structural glasses to plastic crystals, to polymers and colloids<br>- discuss the thermodynamic theory of the free energy of solutions and binary mixtures<br>- use the concept of chemical potential to describe self-assemply in water-surfactant systems<br>- enumerate the main technological applications of molecular and soft condensed matter systems, and discuss the relevance of soft matter to explain biological structure formation and biophysical processes. |
| Examination | Written final exam and homework assignments (problems and case studies)<br>Final mark = Max{FinalExam ; 0.8*FinalExam + 0.2*Homework} |
| Classification | Physics-Chemistry |

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<tr><th colspan="4">TERM 2 – Polytechnic University of Catalonia (UPC) – Spain</th></tr>
<tr><td>Course name</td><td colspan="3">Large facilities: synchrotron and neutron sources</td></tr>
<tr><td>Credit Points (ECTS) 3</td><td>Hours (Face-to Face in class):<br>Lectures: 42<br>Practical works: 3<br>Total: 45</td><td>Duration<br>half semester</td><td>Mode<br>Compulsory (Tracks 1 and 2)</td></tr>
<tr><td>Instructors</td><td colspan="3">P. Bruna, Y. A. Koubychine, L. C. Pardo</td></tr>
<tr><td>Contents</td><td colspan="3">Course syllabus:<br>1. Basics of particle accelerators<br>2. Generation of electromagnetic radiation<br>3. Examples of large facilities: colliders, ion accelerators, synchrotron radiation and spallation sources<br>4. The basics of X-ray and neutron scattering<br>5. Beamlines<br>6. Inelastic neutron scattering<br>7. Neutron applications<br>8. Diffraction at Synchrotron Sources<br>9. Fundamentals of X-ray Absorption Fine Structure (XAFS)<br>10. Hard X-Ray Synchrotron Imaging Techniques and other techniques<br>11. Frequentist data analysis<br>12. Bayesian data analysis</td></tr>
<tr><td>Skills acquired</td><td colspan="3">Students will be able to understand the working principle of neutron and X-ray sources, and to discuss the basics of interaction and scattering of these beams with matter. Students will also acquire knowledge about existing facilities and technical equipment available to manipulate and detect particles and X-rays. In the second part of the course, students will learn which neutron- and synchrotron-radiation- based techniques (including diffraction, X-ray absorption) can be employed for different experimental goals, with particular reference to the type of information that can be extracted from each method. Also imaging methods will be covered. Finally, students will acquire skills on data and errors, and on classical fitting methods, and have hands-on experience on data analysis hypothesis testing and in the practice of model selection.</td></tr>
<tr><td>Examination</td><td colspan="3">The written exams will be multiple choice tests or short exercises that will be carried out during teaching hours once the part of the syllabus to be assessed has been completed. For these individual tests, only a calculator can be used. The exercises, project and practices can be done both individually and in groups. The final mark will consist of the following items (with indicated the percent weight of each):<br>Written exams: 40%<br>Written assignments: 25%<br>Project: 15%<br>Practical work: 20%</td></tr>
<tr><td>Classification</td><td colspan="3">Materials Science</td></tr>
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<tr><th colspan="4">TERM 2 – Polytechnic University of Catalonia (UPC) – Spain</th></tr>
<tr><td>Course name</td><td colspan="3">Biopham short internship</td></tr>
<tr><td>Credit Points (ECTS) 3</td><td>Hours (Face-to Face in class):<br>Lectures: 0<br>Practical works: 45<br>Total: 45</td><td>Duration<br>2 months</td><td>Mode<br>Compulsory (Tracks 1 and 2)</td></tr>
<tr><td>Instructors</td><td colspan="3">The project will have a direct supervisor, who will differ from project to project, and a UPC tutor, in charge of checking that academic duties are fulfilled. The tutor is R. Macovez.</td></tr>
<tr><td>Contents</td><td colspan="3">Research/industrial internship in which the students will carry autonomous research (in an experimental or computational project).</td></tr>
<tr><td>Skills acquired</td><td colspan="3">After completion of the internship, the students will have hands-on, operative knowledge of a research project carried out either at a university, research institute or facility, or private company. They will actively participate in a line of research or development of a product, and become acquainted with the work environment which is the target of the Erasmus Mundus programme.</td></tr>
<tr><td>Examination</td><td colspan="3">The final mark will stem from two evaluations:<br>- Evaluation by Direct Supervisor (80% of the final mark).<br>- Written report evaluated by Tutor (20% of the final mark)</td></tr>
<tr><td>Classification</td><td colspan="3">It will depend on the project, but most Short Intership projects will be in Materials Science, Biophysics, or Physics-Chemistry.</td></tr>
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<tr><th colspan="4">TERM 2 – Polytechnic University of Catalonia (UPC) – Spain</th></tr>
<tr><td>Course name</td><td colspan="3">Machine learning with neural networks</td></tr>
<tr><td>Credit Points<br>(ECTS) 4</td><td>Hours (Face-to Face in class):<br>Lectures: 26<br>Practical works: 10<br>Total: 36</td><td>Duration<br>half semester</td><td>Mode<br>Optional</td></tr>
<tr><td>Instructors</td><td colspan="3">F. Mazzanti, R. Pastor</td></tr>
<tr><td>Contents</td><td colspan="3">Course syllabus:<br>(1) General Concepts of Learning and Neural Networks<br>Students will receive general knowledge related to neural networks, that is, the knowledge common to any type of network, plus the biological and mathematical justification of these concepts. The classification of neural networks will be motivated and the different networks will be described in general terms. The basic concepts of machine learning and its specific implementation associated with neural networks are described (the functionality of a network is achieved through the learning of the network, given some data associated with a specific problem).<br>(2) Feed-forward Neural Networks: Multi-layer Perceptrons, Support Vector Machines and Convolutional Networks.<br>This first block of the course will revolve around feed-forward networks and the Backpropagation training algorithm. The three most commonly used architectures will be explained: The Perceptron and its generalization (Support Vector Machines), the multilayer perceptrons and the convolutional networks. We will emphasize the practical aspects of the subject matter, putting much detail on the problems that may appear when training these networks with real problems. A practice related to the content of this block will be assessed.<br>(3) Recurrent Neural Networks: Hopfield networks, Boltzmann Machines and LSTM<br>This second block of the course will focus on recurrent networks, where we will see Hopfield networks and Boltzmann Machines as classic examples of recurrent network and Restricted Boltzmann Machines (RBM) and the LSTM as examples of networks used in practical problems. A practical work will be done on RBMs learning algorithm, called Contrastive Divergence (CD-k). This part includes and introduction to Deep Learning.</td></tr>
<tr><td>Skills acquired</td><td colspan="3">At the end of part (1), students will be able to explain the concept of Neural Network, describe the different types of network, and the concept and peculiarities of Machine Learning. Students will acquire basic knowledge of Python to understand how neural network and Machine Learning can be implemented.<br>After part (2), students should be able to describe multi-layer perceptions and implement the backpropagation learning algorithm. Students will understanding the mechanism of work of the Rosenblatt Perceptron and of more sophisticated machines (Support Vector Machines)<br>They should be able to give a detailed description of Convolutional Neural Networks, and solve practical problems that may appear in the training of</td></tr>
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| | Neural Networks.<br>Finally, on successful completion of part (3), students will be able to understand:<br>- the difference between a recurrent network and a feed-forward network<br>- the Hopfield model as a simple example of a recurrent network<br>- the Boltzmann Machines (BM) and the concept of learning a distribution of probability<br>- the Boltzmann Restricted Machines (RBM) and the advantages over BMs<br>- the details of the Contrastive Divergence algorithm to train RBMs<br>- the management of sequential data by means of LSTMs<br>Students will also be able to relate the previously mentioned models to Deep Learning |
| Examination | It will be based on two aspects:<br>- Computer assignments<br>- Written final exam |
| Classification | Physics |

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<tr><th colspan="4">TERM 2 – Polytechnic University of Catalonia (UPC) – Spain</th></tr>
<tr><td>Course name</td><td colspan="3">Complexity in biological systems</td></tr>
<tr><td>Credit Points<br>(ECTS) 4</td><td>Hours (Face-to Face in class):<br>Lectures: 32<br>Practical works: 4<br>Total: 36</td><td>Duration<br>half semester</td><td>Mode<br>Optional</td></tr>
<tr><td>Instructors</td><td colspan="3">S. Alonso, A. Pons</td></tr>
<tr><td>Contents</td><td colspan="3">Course syllabus:<br>(1) Complex spatio-temporal dynamics in biology<br>- Oscilations, excitability, bistability<br>- Sinchronization in biological systems<br>- Stochastic biochemistry<br>(2) Analysis of complex biosignals<br>- Deterministic and stochastic signals<br>- Statistical properties<br>- Non-lineal analysis of temporal series<br>(3) Self-organization in biological systems<br>- Excitability and cardiac tissue<br>- Self-assembling: protein folding and membrane formation<br>- Cell polarization, chemotaxis and morphogenesis<br>(4) Biological networks<br>- Introduction to networks<br>- Networks in Biology (examples : metabolic, regulatory and signalling networks ; ecology and epidemiology networks)<br>- Networks in the brain</td></tr>
<tr><td>Skills acquired</td><td colspan="3">At the end of the course, students should be able to:<br>- Understand what a complex system is and how to characterize it<br>- Obtain a basic knowledge of biological phenomena, from the molecular/cellular scale to the macroscale<br>- Dominate numerical techniques and use specific software related with the course<br>- Be able to include the theoretical knowledge to solve biological problems<br>- Be able to present the results of a project in a written text and orally, using a precise language and putting the results in the correct context.</td></tr>
<tr><td>Examination</td><td colspan="3">The final mark for this course will be as follows:<br>Final mark = WT*0.6 + HW*0.4,<br>where WT is the mark of the written test, and HW the mark of homework assignments (applied activities, case studies, problem solving, bibliographic searches, etc.).</td></tr>
<tr><td>Classification</td><td colspan="3">Biophysics</td></tr>
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<tr><th colspan="4">TERM 2 – Polytechnic University of Catalonia (UPC) – Spain</th></tr>
<tr><td>Course name</td><td colspan="3">Stochastic methods for optimization and simulation</td></tr>
<tr><td>Credit Points<br>(ECTS) 4</td><td>Hours (Face-to Face in class):<br>Lectures: 16<br>Practical works: 20<br>Total: 36</td><td>Duration<br>half semester</td><td>Mode<br>Compulsory track 1<br>Optional track 2</td></tr>
<tr><td>Instructors</td><td colspan="3">J. Casulleras, G. Astrakharchik</td></tr>
<tr><td>Contents</td><td colspan="3">Course syllabus:<br>1. Monte Carlo integration: distribution functions and their sampling, crude Monte Carlo, rejection, variance reduction techniques, multidimensional integration, Metropolis method.<br>2. Monte Carlo optimization: simulated annealing, genetic algorithms. Optimal control theory<br>3. Application of Monte Carlo methods to many particles systems. Discrete and continuous systems. Classical simulation of condensed phase systems: simple monoatomic systems, molecular materials, bio-molecules.<br>4. Dynamic Monte Carlo: random paths and diffusion equation, Fokker-Planck and Langevin methods, Brownian dynamics.<br>5. Applications of Monte Carlo methods to quantum systems: wave functions for bosons and fermions, variational Monte Carlo, diffusive Monte Carlo, path integral Monte Carlo.</td></tr>
<tr><td>Skills acquired</td><td colspan="3">At the end of the course, students will have gained:<br>- the ability to generate random numbers according to simple probability distribution laws, and to perform a multidimensional integral using the Monte Carlo method and correctly estimate its statistical variance ;<br>- knowledge of the methods for reducing variance and their optimal choice according to the type of problem to be solved ;<br>- knowledge of the techniques in optimal control theory and the ability to apply Monte Carlo methods to find the optimal solution ;<br>- technical know-how to make a classical simulation of a multiparticle system using the Metropolis method ;<br>- understanding of the basic theory of quantum Monte Carlo, technical know-how to build a Monte Carlo program for the calculation of its properties ;<br>- the ability to perform multidimensional optimization using stochastic techniques, and knowledge of the main stochastic methods used in the study of quantum systems.</td></tr>
<tr><td>Examination</td><td colspan="3">The examination for this course will be based on two types of activities : presentations of practical work in the classroom using computer equipment ; and evaluable written reports. The relative weight for the final mark will be:<br>- Oral presentation 25%<br>- Works carried out by the student 75%</td></tr>
<tr><td>Classification</td><td colspan="3">Physics</td></tr>
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<tr><th colspan="4">TERM 2 – Polytechnic University of Catalonia (UPC) – Spain</th></tr>
<tr><td>Course name</td><td colspan="3">Biophysical and materials science characterization</td></tr>
<tr><td>Credit Points (ECTS) 4</td><td>Hours (Face-to Face in class):<br>Lectures: 30<br>Practical works: 6<br>Total: 36</td><td>Duration<br>half semester</td><td>Mode<br>Compulsory track 2<br>Optional track 1</td></tr>
<tr><td>Instructors</td><td colspan="3">B. Echebarria, T. Pradell</td></tr>
<tr><td>Contents</td><td colspan="3">(1) Physicochemistry of solutions<br>Introduction to inorganic chemical physics of electrolyte & nonelectrolyte solutions: Types of solutions. Thermodynamics of solutions (entropy, free energy and chemical potential; phase diagrams).<br>Properties of water: The hydrogen bond, solubility of molecules in water, polar and non-polar solvents. Electrical permeability of water. Dissociation: acids and bases, protonation.<br>Properties of solutions: functional groups, hydrophilic and hydrophobic interactions; solubility; diffusion. Colligative properties: boiling-point elevation, freezing point depression, osmotic pressure. Surface tension, capillarity. Water phase diagram and anomalies; aqueous electrolytes; non-electrolyte solutions. Electrostatics for salty solutions: biopolymers (polyelectrolytes) and biomembranes in water; Poisson-Boltzmann equation, Debye-Hückel model, electric double layers, ion and proton conduction; transport properties.<br>(2) Applications to pharmaceutics, drug formulation, & biophysical pharmacology<br>- Optical microscopy: bright field, dark field, fluorescence, and confocal microscopy. Super-resolution microscopy<br>- Experimental techniques for electrolyte and non-electrolyte solutions<br>- Small Molecules (drugs): HPLC, Chromatography, Mass spectroscopy, ICP-MS<br>- Characterization of Nanoparticles: Molecular sizes (Dynamics light scattering, DLS), Surface charge (zeta potential, with conductivity measures)<br>- Characterization of Biomolecules: chromatography, gel electrophoresis, Western Blot<br>(3) Physicochemistry of solids<br>Introduction to inorganic solid-state chemical physics (cohesive interactions; organic solids and salts); structural and mechanical properties of homogeneous solids; non-miscible systems: morphology and properties of phase-separated materials<br>(4) Laboratory techniques<br>- Elemental analysis: photoelectron & mass spectroscopy (XPS, UPS, Auger, secondary ion mass spectroscopy)<br>- Chemical analysis: optical and vibrational spectroscopy (UV-vis, IR, Raman), nuclear magnetic resonance (NMR)<br>- Morphological analysis: contact angle, powder X-ray diffraction (XRD), tomography (microCT), NMR-imaging, electron microscopy (SEM, TEM, energy loss/secondary electron spectroscopy)<br>- Phase-change analysis<br>- Mechanical, electrical and optical characterization</td></tr>
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| | - A pharmaceutical application: optical measurement of the dissolution kinetics and solubility of a drug |
| Skills acquired | At the end of the course, students should:<br>- be able to understand the fundamentals of electrolyte and non-electrolyte solutions, including technical literature in this field ;<br>- have knowledge and understanding of different experimental techniques used in biophysical characterization ;<br>- understand the fundamentals of solid-state physical chemistry, including technical literature in this field ;<br>- understand, and know how to use different experimental techniques of materials characterization. |
| Examination | To compute the mark of the course, the professors will consider hand-in exercises (HE), a project during the first part of the course (P), laboratory reports (LR), and a final exam (FE).<br>The final mark (FM) for a student will be calculated according to the formula: FM=0.15*HE+0.2*P+0.35*LR+0.3*FE |
| Classification | Physics-Chemistry |

| TERM 3 – University of Lille (ULille) – France | | | | |
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| **Course name** | **Classification** | **ECTS** | **Hours face-to-face in class** | **Compulsory/optional Recommendation** |
| Advanced thermodynamics and phase transformations | Physics | 3 | 24h | Compulsory |
| Molecular mobility and amorphous state of matter | Physics | 3 | 24h | Compulsory |
| Drug product development and pharmaceutical technology II | Pharmacy | 3 | 24h | Compulsory |
| Thermal analysis of pharmaceuticals | Materials science | 3 | 24h | Compulsory |
| Structural and dynamical characterization of pharmaceuticals | Materials science | 3 | 24h | Compulsory |
| Structural properties of matter: electron microscopy and diffraction | Physics | 3 | 31h | Compulsory |
| Advanced Spectroscopy of Molecular Systems: From Gas Phase to Condensed Matter | Physics | 3 | 27h | Compulsory |
| Atomic scale modeling II – Quantum methods | Physics | 3 | 28h | Compulsory |
| Joint advanced winter course | N/A | 3 | 24h | Compulsory |
| Foreign language (French or English) | N/A | 3 | 24h | Compulsory |
| **TOTAL** | | **30** | **254h** | |

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<tr><th colspan="4">TERM 3 – University of Lille (ULille) – France</th></tr>
<tr><td>Course name</td><td colspan="3">Advanced thermodynamics and phase transformations</td></tr>
<tr><td>Credit Points (ECTS) 3</td><td>Hours (Face-to Face in class):<br>Lectures: 24h<br>Practical works: -<br>Total: 24h</td><td>Duration<br>1 semester</td><td>Mode<br>Compulsory</td></tr>
<tr><td>Instructors</td><td colspan="3">Frédéric Affouard</td></tr>
<tr><td>Contents</td><td colspan="3">The course provides the theoretical basis for understanding equilibrium and out-of-equilibrium condensed physical states and their transformations (crystallization/melting, amorphisation, phase separation) under various stresses (pressure, temperature, milling, dehydration) in a wide range of existing materials (metallic alloys, organic/inorganic glasses, polymers).<br>Course outline<br>• Thermodynamics of single-component systems (reminders): Physical states (crystalline polymorphs and amorphous forms). Stability, metastability, and instability. Calorimetric experimental method to probe transformations.<br>• Thermodynamics of multicomponent systems: Construction and interpretation of binary phase diagrams. Gibbs free energy diagrams as a function of mixture composition. Binodal & spinodal. Precipitations. Eutectic systems. Miscibility, and solubility.<br>• Dynamics of phase transitions: Nucleation and growth. Interfaces. Avrami model. Time-Temperature-Transformation (TTT) diagrams. Spinodal decomposition. Cahn–Hilliard equation.<br>• Thermodynamics of the glassy states and glass transition: Duality crystal vs glass. Kinetic vs thermodynamic transition. Enthalpy, heat capacity and entropy functions in the glass transition region. Kauzmann Paradox. Good and poor glass-forming materials. Conditions for glass formation. Thermal and a-thermal techniques to obtain a glass. Modern theories of glasses.</td></tr>
<tr><td>Skills acquired</td><td colspan="3">On successful completion of the course students will be able to:<br>• To know the different physical states and the transformations of the main classes of existing materials<br>• Construct, describe and interpret a phase diagram from Gibbs energy for single-component and multicomponent systems<br>• Describe the theoretical basis for, be able to formulate and apply classical models for phase transformations (crystallization, melting, vitrification) and be able to make use of this knowledge to carry out relevant quantitative calculations<br>• Know the basic principles of calorimetric techniques for the study of phase transformations</td></tr>
<tr><td>Examination</td><td colspan="3">Written final exam</td></tr>
<tr><td>Classification</td><td colspan="3">Physics</td></tr>
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<tr><th colspan="4">TERM 3 – University of Lille (ULille) – France</th></tr>
<tr><td>Course name</td><td colspan="3">Molecular mobility and amorphous state of matter</td></tr>
<tr><td>Credit Points (ECTS) 3</td><td>Hours (Face-to Face in class):<br>Lectures: 24h<br>Practical works: -<br>Total: 24h</td><td>Duration<br>1 semester</td><td>Mode<br>Compulsory</td></tr>
<tr><td>Instructors</td><td colspan="3">Emeline Dudognon</td></tr>
<tr><td>Contents</td><td colspan="3">This course presents the characteristics of molecular motions found in amorphous materials in the supercooled and glassy states, and the temperature dependence of these dynamics.<br><br>Objectives<br>This course provides an overview of the different types of molecular mobilities characterising the glass-forming liquids and some mesophases (wide amplitude motions, localised motions of intra- or inter- molecular origins), and their properties. It also introduces the main techniques used to characterise these dynamics. The objective is to be able to identify and analyse the different relaxational processes encountered in the glassy and supercooled liquid states.<br><br>Course outline<br>• Introduction: spatial and temporal scales of the different types of motions, fluctuation/dissipation theorem; Short reminders about the different structural organisations of materials (crystals, mesophases, glasses)<br>• Technics allowing the study of molecular mobility: dielectric relaxation spectroscopy, thermo-stimulated currents, dynamic mechanical analysis<br>• Dynamics of glass-forming liquids: main dynamics (fingerprints, non-Arrhenius behaviour and non-exponentiality), secondary relaxations of intra- and inter- molecular origins, relaxations beyond the main relaxation, non-linearity of relaxations in the glassy state, Case studies<br>• Relaxations in semi-crystalline materials and some mesophases</td></tr>
<tr><td>Skills acquired</td><td colspan="3">On successful completion of the course, students will be able to:<br>• identify the different types of glass-forming liquids,<br>• know the basic principles of relaxation spectroscopies (DRS, DMA),<br>• analyse a relaxation spectrum,<br>• construct, describe and interpret an Arrhenius diagram,<br>• identify a dynamic process by the determination of the associated relaxation time, its behaviour law and its activation energy,<br>• make use of their knowledge of relaxational processes to determine the influence of the dynamics on the molecular properties of amorphous materials.</td></tr>
<tr><td>Examination</td><td colspan="3">Written final exam</td></tr>
<tr><td>Classification</td><td colspan="3">Physics</td></tr>
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<tr><th colspan="4">TERM 3 – University of Lille (ULille) – France</th></tr>
<tr><td>Course name</td><td colspan="3">Drug product development and pharmaceutical technology II</td></tr>
<tr><td>Credit Points (ECTS) 3</td><td>Hours (Face-to Face in class):<br>Lectures: 16h<br>Practical works: 8h<br>Total: 24h</td><td>Duration<br>1 semester</td><td>Mode<br>Compulsory</td></tr>
<tr><td>Instructors</td><td colspan="3">Juergen Siepmann (Resp.), Florence Siepmann, Mounira Hamoudi, Youness Karrout, Susanne Florin Muschert</td></tr>
<tr><td>Contents</td><td colspan="3">This course equips students with advanced skills in formulating and manufacturing complex drug delivery systems, including poorly soluble and controlled release products. It combines in-depth theoretical knowledge with hands-on training in modern pharmaceutical technologies and quality control methods.<br>This course focuses on the formulation and manufacturing of complex drug products, especially those with poor water solubility or requiring controlled release. It covers advanced delivery systems like ASDs, SMEDDS, nanocrystals, and biodegradable implants, emphasizing drug release mechanisms and stability issues. Students will explore lab and industrial-scale techniques such as hot melt extrusion and spray-drying, along with strategies to overcome formulation hurdles. Practical training includes preparation methods like drug dissolution testing and film coating. The course integrates theoretical knowledge with hands-on experience to prepare students for real-world pharmaceutical development and manufacturing challenges.<br>This course will address formulation strategies and manufacturing procedures for: (i) more challenging drugs, in particular those exhibiting poor solubility in aqueous media, as well as for (ii) drug products providing controlled release of the active agents over time. This includes for example the formulation and preparation of amorphous solid dispersions (ASDs), Self-Micro-Emulsifying Drug Delivery Systems (SMEDDS), nanocrystals, biodegradable controlled release microparticles and implants, as well as coated dosage forms. Special emphasis will be placed on the underlying drug release mechanisms. Common pitfalls will be treated and hurdles to be faced will be explained. The students will get familiar with the manufacturing techniques that can be used to prepare the different types of dosage forms at the laboratory and industrial scale (e.g. hot melt extrusion, spray-drying). Key risks, such as instability of the drug product during long term storage will be addressed. The students will learn how to aim at overcoming these hurdles. Practical examples will illustrate the application of the formulation and manufacturing strategies for a variety of drug products.<br>This course will also provide practical training on different preparation techniques for drug products (e.g., dissolution testing and film coating) and the most important characterization techniques described in the European and United States Pharmacopoeia. The students will gain a thorough understanding of specific apparatuses which can be used to manufacture drug products and control their quality. They learn how to handle drugs and a variety of excipients. They will get used to measure drug dissolution kinetics. The students will get familiar with different types of equipment and quality control tests, including</td></tr>
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| | those suitable for the manufacturing and characterization of time-controlled drug delivery systems and drug products containing poorly water-soluble drugs. Special emphasis will be placed on common practical pitfalls and challenges. |
| Skills acquired | On successful completion of the course students will:<br>• Identify the potential challenges related to specific drugs and manufacturing procedures<br>• Understand strategies used to formulate poorly soluble drugs<br>• Be familiar with formulation approaches allowing to control drug release over prolonged periods of time<br>• Select the most appropriate preparation methods in the light of the key properties of the drugs<br>• Identify the key hurdles for the formulation development of a specific drug<br>• Differentiate the various preparation methods for drug products, their practical advantages and disadvantages<br>• Know the most adapted experimental techniques to prepare drug products<br>• Apply the key characterization methods for a variety of pharmaceutical dosage forms<br>• Be familiar with the common pitfalls and challenges related to state-of-the-art manufacturing equipment for pharmaceutical products |
| Examination | 1 final oral exam.<br>1 report based on the lab practical session |
| Classification | Pharmacy<br>The courses will be held at the College of Pharmacy (University of Lille). |

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<tr><th colspan="4">TERM 3 – University of Lille (ULille) – France</th></tr>
<tr><td>Course name</td><td colspan="3">Thermal analysis of pharmaceuticals</td></tr>
<tr><td>Credit Points (ECTS) 3</td><td>Hours (Face-to Face in class):<br>Lectures: 12h<br>Practical works: 12h<br>Total: 24h</td><td>Duration<br>1 semester</td><td>Mode<br>Compulsory</td></tr>
<tr><td>Instructors</td><td colspan="3">Natalia Correia (Resp.), Emeline Dudognon, Jean-François Willart</td></tr>
<tr><td>Contents</td><td colspan="3">This course focuses on the thermal techniques to probe the different physical states of pharmaceutical materials and some of their transformations under typical constraints such as temperature changes and milling.<br><br>This course offers a comprehensive presentation of the thermal behaviour of pharmaceutical materials, emphasizing advanced experimental techniques such as Thermogravimetric Analysis (TGA), Differential Scanning Calorimetry (DSC) and Modulated Differential Scanning Calorimetry (MDSC). Students will explore the physical states (crystal, liquid, glass) of pharmaceutical materials (small molecules, polymers) and some their thermal transitions (melting, crystallization, vitrification, dissolution, demixing). Through lectures and practical sessions, the course provides hands-on experience with state-of-the-art analytical tools, enabling students to interpret thermal data critical for drug development and formulation.<br><br>1. Introduction to Thermal Analysis<br>Role of thermal analysis in pharmaceutical development. Overview of thermal behaviour of drug substances and products. Crystalline vs. amorphous states. Polymorphism and its pharmaceutical implications. Physical and chemical transformations: melting, crystallization, glass transition, dissolution, demixing and degradation.<br>2. Thermogravimetric Analysis (TGA)<br>Principles and instrumentation. Applications: moisture content, degradation & degradation kinetics, and compatibility studies.<br>3. Differential Scanning Calorimetry (DSC)<br>Principles and instrumentation. Applications: melting, crystallization, glass transition, and miscibility studies. Interpretation of DSC curves (baseline correction, peak analysis)<br>4. Modulated Differential Scanning Calorimetry (MDSC)<br>Fundamentals of MDSC. Reversible and non-reversible heat flows. Advantages over conventional DSC. Experimental design and best practices. Case studies: detecting subtle transitions, separating overlapping events, amorphous content quantification.</td></tr>
<tr><td>Skills acquired</td><td colspan="3">On successful completion of the course, students will be able to:<br>• Understand the principles of thermal analysis techniques relevant to pharmaceutical materials<br>• Gain proficiency in TGA, standard DSC and MDSC</td></tr>
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| | • Apply thermal analysis data to real-world pharmaceutical challenges |
| Examination | 1 final oral exam.<br>1 report based on the lab practical session |
| Classification | Materials science |

| **TERM 3 – University of Lille (ULille) – France** | | | |
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| Course name | Structural and dynamical characterization of pharmaceuticals | | |
| Credit Points (ECTS) 3 | Hours (Face-to Face in class):<br>Lectures: 12h<br>Practical works: 12h<br>Total: 24h | Duration<br>1 semester | Mode<br>Compulsory |
| Instructors | Natalia Correia (Resp.), Emeline Dudognon, Mathieu Guerain, Frédéric Affouard | | |
| Contents | This course offers an in-depth exploration of complementary advanced experimental techniques—including Raman scattering, Dielectric Relaxation Spectroscopy, optical microscopy, and Powder X-ray diffraction—as well as numerical methods such as Molecular Dynamics, DFT, COSMO-RS, and Machine Learning, all applied to the study of pharmaceutical materials (small molecules and polymers). Students will learn the principles, instrumentation, and applications of these techniques for analysing various physical forms of pharmaceutical materials (drugs and excipients) and for understanding their structural and dynamic characteristics. The course emphasizes extensive laboratory and computer room practice, enabling students to apply these methods effectively in pharmaceutical research.<br><br>1. Introduction to physical states characterization in pharmaceuticals<br>Importance of physical forms in pharmacy. Overview of physical states: crystalline, amorphous, polymorphs, co-crystals. Complementarity of techniques. When and why to combine the techniques.<br>2. Raman Scattering<br>Instrumentation: lasers, optics, detectors. Principle and technique. Advantages and challenges. Applications in pharmaceutical materials & case studies. Polymorph identification and quantification. Mapping and imaging: heterogeneity in formulations.<br>3. Optical Microscopy<br>Instrumentation. Principle and technique. Advantages and challenges.<br>Applications in pharmaceutical materials & case studies. Identifying particle morphology, size distribution, and birefringence. Applications in studying crystallization and phase separation.<br>4. Power X-ray Diffraction (PXRD)<br>Instrumentation. Principle and technique. Advantages and challenges.<br>Applications in pharmaceutical materials & case studies. Structure determination of crystal and co-crystal materials. Phase identification. Crystallinity assessment. Stability studies and solid-state transformations<br>5. Dielectric Relaxation Spectroscopy (DRS)<br>Instrumentation. Principle and technique. Advantages and challenges. Applications in pharmaceutical materials & case studies. Investigations of molecular mobility of glass-forming systems. Glass transition.<br>6. Numerical methods (Molecular Dynamics, DFT, COSMO-RS, Machine Learning)<br>Principle and technique. Advantages and challenges. Complementary with experimental techniques. Applications in pharmaceutical materials & case | | |

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| | studies. Cocrystals computational screening Prediction of the glass-forming ability. Impact of the solvents in nucleation of polymorphs in solution Prediction of mechanical properties |
| Skills acquired | On successful completion of the course, students will be able to:<br>• Understand the principle and complementary of the experimental and numerical techniques.<br>• Gain practical skills in sample preparation, data acquisition, and analysis for each technique.<br>• Apply these techniques to investigate crystal structures, amorphous phases, polymorphism, and microstructure.<br>• Interpret and critically assess experimental data in pharmaceutical contexts.<br>• Recognize the strengths, limitations, and complementary nature of these techniques. |
| Examination | 1 final oral exam.<br>1 report based on the lab practical session |
| Classification | Materials science |

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<tr><th colspan="4">TERM 3 – University of Lille (ULille) – France</th></tr>
<tr><td>Course name</td><td colspan="3">Structural properties of matter: electron microscopy and diffraction</td></tr>
<tr><td>Credit Points (ECTS) 3</td><td>Hours (Face-to Face in class):<br>Lectures: 16h<br>Practical works: 15h<br>Total: 31h</td><td>Duration<br>1 semester</td><td>Mode<br>Compulsory</td></tr>
<tr><td>Instructors</td><td colspan="3">Sébastien Merkel (Resp.), Damien Jacob</td></tr>
<tr><td>Contents</td><td colspan="3">Characterize the state of materials at the crystal to nanometer scale using advanced experimental methods such as the scanning and transmission electron microscope, and powder X-ray diffraction<br>Objectives<br>This course introduces advanced techniques for structural characterization of materials, with a focus on electron microscopy and X-ray diffraction. The student will learn the fundamentals of light-matter interactions, materials characterization with scanning and transmission electron microscope, and powder X-ray diffraction. The course includes hands-on practicals on the SEM and TEM and data processing of powder X-ray diffraction using the Rietveld method.<br>In class courses<br>6h: Introduction to material’s characterization methods, Light-matter interaction, Powder X-ray diffraction and Rietveld implementation<br>10h: Electron microscopy, Electron-matter interactions, Basics of Scanning Electron Microscopy (signals, imaging, chemical analysis, Basics of Transmission) Electron Microscopy (optics, imaging, diffraction, chemical analysis and spectroscopy)<br>In class practicals<br>6h: Powder X-ray diffraction data processing using the Rietveld method<br>3h: TEM data analysis<br>In Labs: 3h SEM, 3h TEM</td></tr>
<tr><td>Skills acquired</td><td colspan="3">• Analysis and interpretation of powder X-ray diffraction data using the Rietveld method<br>• Study of materials properties using the SEM and TEM<br>• Identification, use, and interpretation of advanced experimental methods for the characterization of materials<br>• Develop and conduct complex experiments using advanced technological equipments</td></tr>
<tr><td>Examination</td><td colspan="3">Report on Rietveld analysis<br>Report on Electron microscopy<br>Final exam</td></tr>
<tr><td>Classification</td><td colspan="3">Physics, Materials science</td></tr>
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<tr><th colspan="4">TERM 3 – University of Lille (ULille) – France</th></tr>
<tr><td>Course name</td><td colspan="3">Advanced Spectroscopy of Molecular Systems: From Gas Phase to Condensed Matter</td></tr>
<tr><td>Credit Points (ECTS) 3</td><td>Hours (Face-to Face in class):<br>Lectures: 12h<br>Practical works: 15h<br>Total: 27h</td><td>Duration<br>1 semester</td><td>Mode<br>Compulsory</td></tr>
<tr><td>Instructors</td><td colspan="3">Bertrand Chazallon, Claire Pirim, Emeline Dudognon, Motiyenko Roman</td></tr>
<tr><td>Contents</td><td colspan="3">Characterize<br>This course aims to introduce fundamental principles in molecular physics characterization by optical (vibrational, rotational) and neutron spectroscopies, as well as dielectric techniques.<br><br>This course is situated within the framework of molecular physics and is intended for students pursuing research in molecular spectroscopy, gas-phase and condensed-phase molecular dynamics, and physical chemistry applied to environmental sciences, planetary sciences and pharmaceutics, with a strong physics foundation.<br><br>Objectives<br>• Acquire theoretical understanding and practical insight into advanced spectroscopy methods.<br>• Understand how molecules interact with photons, neutrons, and alternating electric fields.<br>• Analyze and interpret vibrational, rotational, and dielectric spectra.<br>• Connect spectroscopic signatures to the structural and dynamic properties of studied systems.<br><br>Course outline<br>Lecture 1: Optical and Neutron Scattering (Raman and Neutron Spectroscopy)<br>• Principles of inelastic scattering and selection rules.<br>• Experimental setups and spectral interpretation. Applications in environmental science, planetary science, and pharmaceutics.<br>Lecture 2: Absorption Spectroscopy (FTIR)<br>• Dipole-based infrared absorption and selection rules.<br>• Michelson interferometer operation and Fourier analysis.<br>• Identifying functional groups and molecular vibrations; applications across materials.<br>Lecture 3: Microwave Spectroscopy<br>• Rigid rotor model and rotational transitions.<br>• Analyzing rotational spectra to extract molecular parameters.<br>• Applications in astrophysics, atmospheric science, and molecular identification.<br>Lecture 4: Dielectric Spectroscopy<br>• Dielectric response to alternating electric fields.</td></tr>
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|---|---|
| | • Relaxation processes and conductivity spectra.<br>• Applications to disordered systems and slow molecular dynamics. |
| Skills acquired | Direct skills:<br>• Interpret Raman, neutron, FTIR, microwave, and dielectric spectra.<br>• Optimize experimental parameters for specific samples.<br>• Extract molecular information using classical and quantum models.<br>Indirect skills:<br>• Compare light-, particle-, and field-based spectroscopic methods.<br>• Identify relevant techniques for addressing molecular-level questions in various phases.<br>• Understand the relationship between microstructure and spectroscopic signatures |
| Examination | Written exam<br>Reports on practical on research instruments |
| Classification | Physics |

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<tr><th colspan="4">TERM 3 – University of Lille (ULille) – France</th></tr>
<tr><td>Course name</td><td colspan="3">Atomic scale modeling II – Quantum methods</td></tr>
<tr><td>Credit Points (ECTS) 3</td><td>Hours (Face-to Face in class):<br>Lectures: 16h<br>Practical works: 12h<br>Total: 28h</td><td>Duration<br>1 semester</td><td>Mode<br>Compulsory</td></tr>
<tr><td>Instructors</td><td colspan="3">Denis Duflot (Resp.), Philippe Carrez, Pierre Hirel</td></tr>
<tr><td>Contents</td><td colspan="3">Discover quantum first principles methods to solve the problem of the electronic structure of molecular systems, from isolated molecules to solids<br><br>Objectives<br>• Identify when and why to use quantum methods for research problems<br>• Find stable equilibrium structures.<br>• Calculate relevant physical and/or chemical properties<br><br>Course outline<br>• The electronic structure problems for molecular systems: how to solve the Schrödinger equation?<br>• The Hartree-Fock approximation<br>• Linear Combination of Atomic Orbitals and basis sets, pseudo-potentials<br>• Semi-empirical methods; from Hückel to DFTB<br>• Beyond Hartree-Fock : the correlation problem<br>• Basics of post-Hartree Fock methods<br>• Density Functional Theory (DFT): basic concepts and application to molecules and solids<br>• Hybrid methods: combine quantum and classical techniques for large systems</td></tr>
<tr><td>Skills acquired</td><td colspan="3">By completing this lecture, students will gain the ability to:<br>• Choose appropriate level of theory to solve problems: accuracy versus computational cost<br>• Get geometries of molecular and solid structures using energy minimization techniques.<br>• Calculate spectroscopic properties: Infrared and Raman spectra, band structure, phonons<br>• Introduction to reactivity: get transition state structures, evaluate reaction rates</td></tr>
<tr><td>Examination</td><td colspan="3">Report and oral defense</td></tr>
<tr><td>Classification</td><td colspan="3">Physics</td></tr>
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