



Livret pédagogique

**M2 - ADVANCED PHYSICS
OF PHARMACEUTICAL
MATERIALS**

2026 - 2027

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Contacts

Objectives and content of the training :

The A2PM master track seeks to provide students with a comprehensive understanding of physics of materials its multifaceted applications in pharmacy. The programme integrates core disciplines such as physics, materials science and pharmacy. It leverages the specialties and research strengths to offer a multidisciplinary and innovative curriculum. A2PM applies fundamental physical principles common in materials science to address challenges in areas such as: Drug delivery systems, manipulation of physical states of drug forms, manufacturing and processing of nanoscopic and microscopic particle systems, structure and properties of bulk powders and their assemblies (e.g., tablets), or improving the stability of dried protein drugs for pharmaceutical applications. The programme offers a comprehensive curriculum that balances theoretical knowledge and practical application.

The master's programme is organised into different knowledge and skills blocks (BCC):

- BCC - Implement fundamental physics tools and approaches to produce highly specialised knowledge;
- BCC - Produce and communicate highly specialised knowledge, including in a professional context related to the field of physics;
- BCC - Solving complex problems by applying fundamental physics concepts

Prerequisites and Target Audience :

Undergraduate students in physics, physico-chemistry and materials science

Educational, technical, and supervisory resources :

The teaching staff consists of professors and faculty members who are also researchers

FORMATION OUVERTE EN FORMATION INITIALE :

	IN CLASS HOURS	ECTS
SEMESTRE 3	230	30
BCC - IMPLEMENTING FUNDAMENTAL PHYSICS TOOLS AND APPROACHES TO PRODUCE HIGHLY SPECIALISED KNOWLEDGE	72	9
UE - Drug product development and pharmaceutical technology II	24	3
EC - Drug product development and pharmaceutical technology II 16h CM/TD - 8h TP		
UE - Thermal analysis of pharmaceuticals	24	3
EC - Thermal analysis of pharmaceuticals 12h CM/TD - 12h TP		
UE - Structural and dynamical characterization of pharmaceuticals	24	3
EC - Structural and dynamical characterization of pharmaceuticals 12h CM/TD - 12h TP		
BCC - PRODUCING AND COMMUNICATING HIGHLY SPECIALIZED KNOWLEDGE, INCLUDING IN A PROFESSIONAL CONTEXT	24	6
UE - Foreign language (1 choice)	24	3
EC - FLE/FOU 24h TD		
EC - Anglais 12h TD		
UE - Winter School	N/A	3
EC - Winter School 0h TD		
BCC - SOLVING COMPLEX PROBLEMS BY APPLYING FUNDAMENTAL PHYSICS CONCEPTS	134	15
UE - Advanced thermodynamics and phase transformations	24	3
EC - Advanced thermodynamics and phase transformations 24h CM/TD		
UE - Molecular mobility and amorphous state of matter	24	3
EC - Molecular mobility and amorphous state of matter 24h CM/TD		
UE - Structural properties of matter : electron microscopy and diffraction	31	3
EC - Structural properties of matter : electron microscopy and diffraction 16h CM/TD - 9h TD - 6h TP		
UE - Atomic scale modeling II - Quantum methods	28	3
EC - Atomic scale modeling II - Quantum methods 16h CM/TD - 12h TP		
UE - Advanced spectroscopy of molecular systems : From gas phase to condensed matter (ASMS)	27	3

EC - Advanced spectroscopy of molecular systems : From gas phase to condensed matter (ASMS) 12h CM/TD - 15h TP		
	IN CLASS HOURS	ECTS
SEMESTRE 4	N/A	30
BCC - PRODUCING AND COMMUNICATING HIGHLY SPECIALIZED KNOWLEDGE, INCLUDING IN A PROFESSIONAL CONTEXT	N/A	30
UE - Internship	N/A	30
EC - Internship 0h TD		

TOTAL IN CLASS HOURS : 230H

BCC : IMPLEMENTING FUNDAMENTAL PHYSICS TOOLS AND APPROACHES TO PRODUCE HIGHLY SPECIALIZED KNOWLEDGE

By implementing advanced and specialized uses of digital tools
 By analyzing data for fundamental physics
 By practicing an experimental approach adapted to a physics problem
 By mobilizing and producing highly specialized knowledge

MASTER 2

ESSENTIAL LEARNING OUTCOMES:

Level of development

Develop and conduct complex experiments using high-tech equipment

Conduct research and scientific studies in materials and molecular physics

Level of autonomy

Use advanced digital tools for materials and molecular physics independently

Propose a robust experimental protocol adapted to a complex problem in materials and molecular physics

SEMESTRE 3

- **UE - Drug product development and pharmaceutical technology II** – 3 ECTS
 - *Drug product development and pharmaceutical technology II*
- **UE - Thermal analysis of pharmaceuticals** – 3 ECTS
 - *Thermal analysis of pharmaceuticals*
- **UE - Structural and dynamical characterization of pharmaceuticals** – 3 ECTS
 - *Structural and dynamical characterization of pharmaceuticals*

Grading rule for this BCC :

In general, the following rules apply to this program:

1. Compensation applies within a BCC (Bloc de Connaissances et de Compétences). A BCC is awarded if the average of the grades obtained in that BCC is equal to or higher than 10.
2. The grade for a BCC is calculated as a weighted average of the corresponding EC (Éléments Constitutifs) and EU (Enseignements Unitaires), with weights proportional to the ECTS credits assigned to each.
3. Unless decided otherwise by the jury, there is no compensation between BCCs or between semesters. Each bcc and each semestre must be validated.
4. Reports, practical work, and oral exams do not have a second session. A replacement solution will be offered for justified absences or delays.
5. For ECs with a final exam, students may choose to take a second session (regardless of their first-session grade). In this case, they assume to cancel their first-session grade which will be replaced with that of the second session. Students with a justified absence for the first session will take their exam in the second session.

The detailed evaluation procedures for each EC and EU are defined below.

BCC : PRODUCING AND COMMUNICATING HIGHLY SPECIALIZED KNOWLEDGE, INCLUDING IN A PROFESSIONAL CONTEXT

By mobilizing and producing highly specialized knowledge
By implementing specialized communication for knowledge transfer
By contributing to transformation in a professional context

MASTER 2

ESSENTIAL LEARNING OUTCOMES:

Level of development

Communicate for training or knowledge transfer purposes, both orally and in writing, in a foreign language.

Manage complex, unpredictable professional or academic contexts that require new strategic approaches.

Respect the principles of ethics, professional conduct, and social and environmental responsibility.

Supervise and carry out research and scientific studies in physics.

Promote and disseminate the results of studies in physical sciences (technical and scientific reports, patent files) within the company and to the scientific community.

Level of autonomy

Develop critical awareness of knowledge in a field and/or at the interface of several fields

Lead a project (design, management, team coordination, implementation and management, evaluation, dissemination) that may require multidisciplinary skills in a collaborative setting

Analyze the technical, environmental, societal, and scientific challenges of projects involving physical phenomena and propose strategies that take into account their potential applications

SEMESTRE 3

- **UE - Foreign language (1 choix) – 3 ECTS**
 - FLE/FOU
 - Anglais
- **UE - Winter School – 3 ECTS**
 - Winter School

SEMESTRE 4

- **UE - Internship – 30 ECTS**
 - Internship

Grading rule for this BCC :

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2. The grade for a BCC is calculated as a weighted average of the corresponding EC (Éléments Constitutifs) and EU (Enseignements Unitaires), with weights proportional to the ECTS credits assigned to each.

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5. For ECs with a final exam, students may choose to take a second session (regardless of their first-session grade). In this case, they assume to cancel their first-session grade which will be replaced with that of the second session. Students with a justified absence for the first session will take their exam in the second session.

The detailed evaluation procedures for each EC and EU are defined below.

BCC : SOLVING COMPLEX PROBLEMS BY APPLYING FUNDAMENTAL PHYSICS CONCEPTS

By mobilizing and producing highly specialized knowledge

By solving complex problems using fundamental concepts of fundamental physics

MASTER 2

ESSENTIAL LEARNING OUTCOMES:

Level of development

Solving problems to develop new knowledge and procedures in materials and molecular physics

Integrating knowledge from different fields

Level of autonomy

Develop critical awareness of knowledge in a field and/or at the interface of several fields

Identify the limitations of models and theories used to address a complex problem

SEMESTRE 3

- **UE - Advanced thermodynamics and phase transformations** – 3 ECTS
 - *Advanced thermodynamics and phase transformations*
- **UE - Molecular mobility and amorphous state of matter** – 3 ECTS
 - *Molecular mobility and amorphous state of matter*
- **UE - Structural properties of matter : electron microscopy and diffraction** – 3 ECTS
 - *Structural properties of matter : electron microscopy and diffraction*
- **UE - Atomic scale modeling II - Quantum methods** – 3 ECTS
 - *Atomic scale modeling II - Quantum methods*
- **UE - Advanced spectroscopy of molecular systems : From gas phase to condensed matter (ASMS)** – 3 ECTS
 - *Advanced spectroscopy of molecular systems : From gas phase to condensed matter (ASMS)*

Grading rule for this BCC :

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that of the second session. Students with a justified absence for the first session will take their exam in the second session.

The detailed evaluation procedures for each EC and EU are defined below.

SEMESTRE 3

DRUG PRODUCT DEVELOPMENT AND PHARMACEUTICAL TECHNOLOGY II

UE : DRUG PRODUCT DEVELOPMENT AND PHARMACEUTICAL TECHNOLOGY II

BCC : IMPLEMENTING FUNDAMENTAL PHYSICS TOOLS AND APPROACHES TO PRODUCE
HIGHLY SPECIALIZED KNOWLEDGE

Class: mandatory

Teaching method: in person

Teaching language: English

Person in charge : Juergen Siepmann – juergen.siepmann@univ-lille.fr

Teaching team : Juergen Siepmann, Florence Siepmann, Mounira Hamoudi, Youness Karrouit, Susanne Florin Muschert

Required prior teaching unit(s):

Suggested readings:

Syllabus :

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.

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.

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.

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 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.

On successful completion of the course students will:

- Identify the potential challenges related to specific drugs and manufacturing procedures
- Understand strategies used to formulate poorly soluble drugs
- Be familiar with formulation approaches allowing to control drug release over prolonged periods of time
- Select the most appropriate preparation methods in the light of the key properties of the drugs
- Identify the key hurdles for the formulation development of a specific drug
- Differentiate the various preparation methods for drug products, their practical advantages and disadvantages
- Know the most adapted experimental techniques to prepare drug products
- Apply the key characterization methods for a variety of pharmaceutical dosage forms
- Be familiar with the common pitfalls and challenges related to state-of-the-art manufacturing equipment for pharmaceutical products

The courses will be held at the College of Pharmacy (University of Lille).

Evaluation methods

1 final oral exam (75%)

1 report based on the lab practical session (25%)

Solution will be offered for justified absences or delays.

THERMAL ANALYSIS OF PHARMACEUTICALS

UE : THERMAL ANALYSIS OF PHARMACEUTICALS

BCC : IMPLEMENTING FUNDAMENTAL PHYSICS TOOLS AND APPROACHES TO PRODUCE
HIGHLY SPECIALIZED KNOWLEDGE

Class: mandatory

Teaching method: in person

Teaching language: English

Person in charge : *Natalia Correia* – natalia.correia@univ-lille.fr

Teaching team : *Natalia Correia, Emeline Dudognon, Jean-François Willart*

Required prior teaching unit(s):

Suggested readings:

Syllabus :

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.

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.

1. Introduction to Thermal Analysis

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.

2. Thermogravimetric Analysis (TGA)

Principles and instrumentation. Applications: moisture content, degradation & degradation kinetics, and compatibility studies.

3. Differential Scanning Calorimetry (DSC)

Principles and instrumentation. Applications: melting, crystallization, glass transition, and miscibility studies. Interpretation of DSC curves (baseline correction, peak analysis)

4. Modulated Differential Scanning Calorimetry (MDSC)

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.

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

- Understand the principles of thermal analysis techniques relevant to pharmaceutical materials
- Gain proficiency in TGA, standard DSC and MDSC
- Apply thermal analysis data to real-world pharmaceutical challenges

Evaluation methods

1 oral exam (2/3)

1 written exam (1/3)

Solution will be offered for justified absences.

STRUCTURAL AND DYNAMICAL CHARACTERIZATION OF PHARMACEUTICALS

UE : STRUCTURAL AND DYNAMICAL CHARACTERIZATION OF PHARMACEUTICALS

BCC : IMPLEMENTING FUNDAMENTAL PHYSICS TOOLS AND APPROACHES TO PRODUCE HIGHLY SPECIALIZED KNOWLEDGE

Class: mandatory

Teaching method: in person

Teaching language: English

Person in charge: Natalia Correia – natalia.correia@univ-lille.fr

Teaching team : Natalia Correia, Emeline Dudognon, Mathieu Guerain, Frédéric Affouard, Timothée Devergne

Required prior teaching unit(s):

Suggested readings:

Syllabus :

This course focuses on complementary experimental and numerical techniques to probe the different physical states of pharmaceutical materials and their transformations

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.

1. Introduction to physical states characterization in pharmaceuticals

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.

2. Raman Scattering

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.

3. Optical Microscopy

Instrumentation. Principle and technique. Advantages and challenges. Applications in pharmaceutical materials & case studies. Identifying particle morphology, size distribution, and birefringence. Applications in studying crystallization and phase separation.

4. Power X-ray Diffraction (PXRD)

Instrumentation. Principle and technique. Advantages and challenges. Applications in pharmaceutical materials & case studies. Structure determination of crystal and co-crystal materials. Phase identification. Crystallinity assessment. Stability studies and solid-state transformations.

5. Dielectric Relaxation Spectroscopy (DRS)

Instrumentation. Principle and technique. Advantages and challenges. Applications in pharmaceutical materials & case studies. Investigations of molecular mobility of glass-forming systems. Glass transition.

6. Numerical methods (Molecular Dynamics, DFT, COSMO-RS, Machine Learning)

Principle and technique. Advantages and challenges. Complementary with experimental techniques. Applications in pharmaceutical materials & case studies. Cocrystals computational screening Prediction of the glass-forming ability. Impact of the solvents in nucleation of polymorphs in solution Prediction of mechanical properties.

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

- Understand the principle and complementary of the experimental and numerical techniques.
- Gain practical skills in sample preparation, data acquisition, and analysis for each technique.
- Apply these techniques to investigate crystal structures, amorphous phases, polymorphism, and microstructure.
- Interpret and critically assess experimental data in pharmaceutical contexts.
- Recognize the strengths, limitations, and complementary nature of these techniques.

Evaluation methods

1 oral exam (2/3)

1 written exam (1/3)

Solution will be offered for justified absences.

FLE / FOU

UE : FOREIGN LANGUAGE

BCC : PRODUCING AND COMMUNICATING HIGHLY SPECIALIZED KNOWLEDGE, INCLUDING
IN A PROFESSIONAL CONTEXT

Class: mandatory

Teaching method: in person

Teaching language: French

Person in charge: Leonore Bereksi – leonore.bereksi@univ-lille.fr

Required prior teaching unit(s): None (a placement test is conducted before the start of the course to assign students to the appropriate level group).

Suggested readings: Depending on the level: Édito student's book, Didier FLE; Grammaire progressive du français, CLE International.

Syllabus :

Dedicated Moodle space for the class group: course progression and materials provided according to the group's level (from A1.1 to B2/C1).

Objectives and skills

(depending on the level group, A1–A2)

Be able to understand concrete situations in everyday life in the present tense; describe current or past events and experiences, as well as future plans; carry out simple administrative procedures; and express a simple opinion.

Listening

Can understand expressions and vocabulary related to matters of immediate personal relevance, particularly in the university context: oneself and one's immediate environment. Can understand the main points of simple and clear messages.

Reading

Can read short, simple texts. Can find specific information in a document and understand short, simple personal correspondence.

Spoken production

Can use a series of phrases and expressions to describe, in simple terms, their family and other people, their living conditions, particularly in a university environment, etc.

Spoken interaction

Can communicate during simple tasks requiring a straightforward exchange of information on familiar topics or activities. Can take part in a brief exchange.

Writing

Can write short, simple notes and messages. Can write a short, simple personal letter or message.

Vocabulary range

The learner uses basic structures consisting of memorised expressions, short groups of words, and ready-made phrases in order to communicate information.

Evaluation procedure

Continuous assessment: 4 grades evaluating written and oral skills, with equal weighting.

Depending on the level group (from A1.1 to B2C1):

- 2 oral grades (1 oral presentation with multimedia support, 1 grade for interaction)

- 2 written grades (2 written assignments)

ANGLAIS

UE : FOREIGN LANGUAGE

BCC : PRODUCING AND COMMUNICATING HIGHLY SPECIALIZED KNOWLEDGE, INCLUDING
IN A PROFESSIONAL CONTEXT

Class: mandatory

Teaching method: in person

Teaching language: English

Person in charge: Karen Becquet karen.becquet@univ-lille.fr

Required prior teaching unit(s):

Suggested readings:

Syllabus :

- Scientific networking, introducing field of work & professional objectives through group discussion
- Practical writing exercises, comparison of different registers
- Technical presentations in Physics : presenting data, concepts, explaining visuals, experimental procedures, responding to questions

Learning outcomes :

By the end of the course, students should be able to:

- Communicate complex physics or maths concepts fluently and accurately in spoken English.
- Present scientific results clearly to non-specialist audiences.
- Reflect on strategies to use appropriate language and register, in both written

Evaluation procedure

Writing (20%) + Oral Presentation (40%) + Interview (40%)

WINTER SCHOOL

UE : WINTER SCHOOL

BCC : PRODUCING AND COMMUNICATING HIGHLY SPECIALIZED KNOWLEDGE, INCLUDING
IN A PROFESSIONAL CONTEXT

Class: mandatory

Teaching method: in person, possible also on-line

Teaching language: English

Person in charge: *Frédéric Affouard* – frederic.affouard@univ-lille.fr

Required prior teaching unit(s):

Suggested readings:

Syllabus :

The programme is designed to provide students with a comprehensive learning experience on topics not typically taught in the classroom.

It will feature:

- Advanced lectures on material sciences, pharmaceuticals, and biomaterials for health applications
- Industry-focused sessions led by professionals on formulation development, manufacturing technologies, and the challenges of industrial scale-up
- Workshops introducing Open Science practices, the FAIR principles (Findable, Accessible, Interoperable, Reusable), as well as topics such as inclusion, diversity, gender equality, dissemination, communication, and public engagement
- Business, strategy, and innovation modules to strengthen career readiness

Beyond the academic content, the winter course is also designed to foster strong interactions among students, professors, invited scholars, and industry experts, who will contribute through lectures and specialized courses.

Ultimately, this event will help students to expand their networks and strengthen their preparation for future careers.

Evaluation procedure

1 final exam

Solution will be offered for justified absences.

ADVANCED THERMODYNAMICS AND PHASE TRANSFORMATIONS

UE : ADVANCED THERMODYNAMICS AND PHASE TRANSFORMATIONS

BCC : SOLVING COMPLEX PROBLEMS BY APPLYING FUNDAMENTAL PHYSICS CONCEPTS

Class: mandatory

Teaching method: in person

Teaching language: English

Person in charge : *Frédéric Affouard* – frederic.affouard@univ-lille.fr

Required prior teaching unit(s):

Suggested readings:

Syllabus :

This course explores the principles governing crystalline and amorphous physical states and their transformations across diverse materials like metallic alloys, glasses, and polymers.

Objectives

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).

Course outline

- Thermodynamics of single-component systems (reminders): Physical states (crystalline polymorphs and amorphous forms). Stability, metastability, and instability. Calorimetric experimental method to probe transformations.
- 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.
- Dynamics of phase transitions: Nucleation and growth. Interfaces. Avrami model. Time-Temperature-Transformation (TTT) diagrams. Spinodal decomposition. Cahn–Hilliard equation.
- 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.

Acquired skills

On successful completion of the course students will be able to:

- To know the different physical states and the transformations of the main classes of existing materials
- Construct, describe and interpret a phase diagram from Gibbs energy for single-component and multicomponent systems

- 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
- Know the basic principles of calorimetric techniques for the study of phase transformations

Evaluation procedure

1 final written exam, 3h

Students may choose to take a second session (regardless of their first-session grade) for the written exam. In this case, they assume to cancel their first-session grade which will be replaced with that of the second session. Students with a justified absence for the first session of the written exam will take their exam in the second session.

MOLECULAR MOBILITY AND AMORPHOUS STATE OF MATTER

UE : MOLECULAR MOBILITY AND AMORPHOUS STATE OF MATTER

BCC : SOLVING COMPLEX PROBLEMS BY APPLYING FUNDAMENTAL PHYSICS CONCEPTS

Class: mandatory

Teaching method: in person

Teaching language: English

Person in charge : *Emeline Dudognon* – emeline.dudognon@univ-lille.fr

Required prior teaching unit(s):

Suggested readings:

Syllabus :

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.

Objectives

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.

Course outline

- 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)
- Technics allowing the study of molecular mobility: dielectric relaxation spectroscopy, thermally stimulated currents, dynamic mechanical analysis
- 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
- Relaxations in semi-crystalline materials and some mesophases.

Acquired skills

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

- identify the different types of glass-forming liquids,
- know the basic principles of relaxation spectroscopies (DRS, DMA),
- analyse a relaxation spectrum,
- construct, describe and interpret an Arrhenius diagram,
- identify a dynamic process by the determination of the associated relaxation time, its behaviour law and its activation energy,
- make use of their knowledge of relaxational processes to determine the influence of the dynamics on the molecular properties of amorphous materials.

Evaluation procedure

2h final written exam

Students may choose to take a second session (regardless of their first-session grade) for the written exam. In this case, they assume to cancel their first-session grade which will be replaced with that of the second session. Students with a justified absence for the first session of the written exam will take their exam in the second session

STRUCTURAL PROPERTIES OF MATTER : ELECTRON MICROSCOPY AND DIFFRACTION

UE : STRUCTURAL PROPERTIES OF MATTER : ELECTRON MICROSCOPY AND
DIFFRACTION

BCC : SOLVING COMPLEX PROBLEMS BY APPLYING FUNDAMENTAL PHYSICS CONCEPTS

Class: mandatory

Teaching method: in person

Teaching language: English

Person in charge : Sébastien Merkel – sebastien.merkel@univ-lille.fr

Teaching team : S. Merkel, D. Jacob

Required prior teaching unit(s):

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Suggested readings:

Syllabus :

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

Objectives

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.

Course outline

In class courses

- 6 h-CM:
 - Introduction to material's characterization methods,
 - Light-matter interaction,
 - Powder X-ray diffraction and Rietveld implementation
- 10 h-CM: 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

In class practicals

- 6 h-TD : Powder X-ray diffraction data processing using the Rietveld method
- 3 h-TD : TEM data analysis

Labs, as small groups

- 3h SEM
- 3h TEM

Acquired skills

- Analysis and interpretation of powder X-ray diffraction data using the Rietveld method
- Study of materials properties using the SEM and TEM
- Identification, use, and interpretation of advanced experimental methods for the characterization of materials
- Develop and conduct complex experiments using advanced technological equipments

Evaluation procedure

Report on Rietveld analysis (1/3)
Report on Electron microscopy (1/3)
Final oral interrogation (1/3)

A solution will be offered for justified absences or delays.

ATOMIC SCALE MODELING II – QUANTUM METHODS

UE : ATOMIC SCALE MODELING II – QUANTUM METHODS

BCC : SOLVING COMPLEX PROBLEMS BY APPLYING FUNDAMENTAL PHYSICS CONCEPTS

Class: mandatory

Teaching method: in person

Teaching language: English

Person in charge : Denis Duflot – denis.duflot@univ-lille.fr

Teaching team : Denis Duflot, Philippe Carrez, Pierre Hirel

Required prior teaching unit(s): Atomic scale modeling I

Suggested readings:

Syllabus :
Discover quantum first principles methods to solve the problem of the electronic structure of molecular systems, from isolated molecules to solids Objectives - Identify when and why to use quantum methods for research problems - Find stable equilibrium structures. - Calculate relevant physical and/or chemical properties Course outline - The electronic structure problems for molecular systems: how to solve the Schrödinger equation? - The Hartree-Fock approximation - Linear Combination of Atomic Orbitals and basis sets, pseudo-potentials - Semi-empirical methods; from Hückel to DFTB - Beyond Hartree-Fock : the correlation problem - Basics of post-Hartree Fock methods - Density Functional Theory (DFT): basic concepts and application to molecules and solids - Hybrid methods : combine quantum and classical techniques for large systems Acquired skills By completing this lecture, students will gain the ability to: - Choose appropriate level of theory to solve problems: accuracy versus computational cost - Get geometries of molecular and solid structures using energy minimization techniques. - Calculate spectroscopic properties: Infrared and Raman spectra, band structure, phonons Introduction to reactivity: get transition state structures, evaluate reaction rates
Evaluation procedure
Report (1/2) and oral defense (1/2) A solution will be offered for justified absences or delays.

ADVANCED SPECTROSCOPY OF MOLECULAR SYSTEMS: FROM GAS PHASE TO CONDENSED MATTER (ASMS)

UE : ADVANCED SPECTROSCOPY OF MOLECULAR SYSTEMS: FROM GAS PHASE TO CONDENSED MATTER (ASMS)

BCC : SOLVING COMPLEX PROBLEMS BY APPLYING FUNDAMENTAL PHYSICS CONCEPTS

Class: mandatory

Teaching method: in person

Teaching language: English

Person in charge: Claire Pirim claire.pirim@univ-lille.fr

Teaching team : Bertrand Chazallon bertrand.chazallon@univ-lille.fr, Claire Pirim claire.pirim@univ-lille.fr,

Dudognon Emeline emeline.dudognon@univ-lille.fr, Motiyenko Roman roman.motiienko@univ-lille.fr

Required prior teaching unit(s):

Suggested readings:

Syllabus :

This course aims to introduce fundamental principles in molecular physics characterization by optical (vibrational, rotational) and neutron spectroscopies, as well as dielectric techniques.

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 pharmaceuticals, with a strong physics foundation.

Objectives

- Acquire theoretical understanding and practical insight into advanced spectroscopy methods.
- Understand how molecules interact with photons, neutrons, and alternating electric fields.
- Analyze and interpret vibrational, rotational, and dielectric spectra.
- Connect spectroscopic signatures to the structural and dynamic properties of studied systems.

Course outline

Lecture 1: Optical and Neutron Scattering (Raman and Neutron Spectroscopy)

- Principles of inelastic scattering and selection rules.
- Experimental setups and spectral interpretation.

Lecture 2: Absorption Spectroscopy (FTIR)

- Dipole-based infrared absorption and selection rules.
- Michelson interferometer operation and Fourier analysis.
- Identifying functional groups and molecular vibrations;
- Applications in environmental and planetary sciences, and pharmaceutical sciences.

Lecture 3: Microwave Spectroscopy

- Rigid rotor model and rotational transitions.

- Analyzing rotational spectra to extract molecular parameters.
- Applications in astrophysics, atmospheric science, and molecular identification.

Lecture 4: Dielectric Spectroscopy

- Dielectric response to alternating electric fields.
- Relaxation processes and conductivity spectra.
- Applications to disordered systems and slow molecular dynamics.

Acquired skills

Direct skills:

- Interpret Raman, neutron, FTIR, microwave, and dielectric spectra.
- Optimize experimental parameters for specific samples.
- Extract molecular information using classical and quantum models.

Indirect skills:

- Compare light-, particle-, and field-based spectroscopic methods.
- Identify relevant techniques for addressing molecular-level questions in various phases.
- Understand the relationship between microstructure and spectroscopic signatures

Evaluation procedure

Written exam (75%) + reports on practical on research instruments (25%)

Students may choose to take a second session (regardless of their first-session grade) for the written exam. In this case, they assume to cancel their first-session grade which will be replaced with that of the second session. Students with a justified absence for the first session of the written exam will take their exam in the second session.

A solution will be offered for justified absences or delays with the reports.

SEMESTRE 4

INTERNSHIP

UE : INTERNSHIP

BCC : PRODUCING AND COMMUNICATING HIGHLY SPECIALIZED KNOWLEDGE, INCLUDING
IN A PROFESSIONAL CONTEXT

Class: **by choice**

Teaching method: **in person**

Teaching language: **Not applicable**

Person in charge : *Frédéric Affouard* – frederic.affouard@univ-lille.fr

Required prior teaching unit(s):

Suggested readings:

Syllabus :

This course is designed to enable students to:

- Immerse themselves in the professional environment of the program
- Apply the theoretical, technical, and methodological knowledge acquired during the program
- Deepen their understanding of the professional environment

Intership - Skills

- Theoretical Skills

- Understanding how the work in a professional environment, either in the private or public research environment

- Technical and Professional Skills

- Develop independence, adaptability, and a sense of responsibility
- Comply with health, safety, and traceability regulations
- Integrate into a workplace team
- Take initiative in managing assigned tasks
- Be able to report on one's work and self-evaluate
- Learn to manage time and follow internal guidelines and procedures

This mandatory internship, consisting of at least 4 months will take place between January and August. It will include the writing of a report and an oral defense. The internship may be completed in France or abroad, in a university laboratory or at a company, and must be conducted under a formal agreement.

Evaluation procedure

Grade from tutor: 30%, grade for report: 20%, grade for oral defense: 50%

A solution will be offered for justified absences or delays with the report or defense.



Campus Cité scientifique

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