



Livret pédagogique

**M1 - ADVANCED PHYSICS
OF PHARMACEUTICAL
MATERIALS**

2026 - 2027

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Contacts

Objectifs et contenus de la formation :

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, chemistry 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 1	255	30
BCC - IMPLEMENTING FUNDAMENTAL PHYSICS TOOLS AND APPROACHES TO PRODUCE HIGHLY SPECIALISED KNOWLEDGE	96	12
UE - States of Matter and Materials Science Primers	24	3
EC - States of Matter and Materials Science Primers 24h CM/TD		
UE - Introduction to Pharmaceutical Materials Science	48	6
EC - Introduction to Pharmaceutical Materials Science 44h TD - 4h TP		
UE - Drug product development and pharmaceutical technology I	24	3
EC - Drug product development and pharmaceutical technology I 16h TD - 8h TP		
BCC - PRODUCING AND COMMUNICATING HIGHLY SPECIALIZED KNOWLEDGE, INCLUDING IN A PROFESSIONAL CONTEXT	62	9
UE - Foreign language (1 choice)	24	3
EC - FLE/FOU 24h TD		
EC - Anglais 18h TD		
UE - GP : Materials for a Sustainable Future	20	3
EC - Materials for a sustainable future 20h TD		
UE - Tutored trainings	18	3
EC - Tutored trainings 4,5h CM/TD - 4,5h TD - 9h TP		
EC - Tutored trainings - Suivi 0h TD		
BCC - SOLVING COMPLEX PROBLEMS BY APPLYING FUNDAMENTAL PHYSICS CONCEPTS	97	9
UE - Continuum mechanics	24	3
EC - Continuum mechanics 24h CM/TD		
UE - AI and advanced computational methods in physics	25	3
EC - AI and advanced computational 10h CM/TD – 15h TP		

UE - Atomic scale modeling I – Classical methods	28	3
EC - Atomic scale modeling I – Classical methods 12h CM/TD – 16h TP		
UE - Remediation	20	0
EC - Remediation 20h CM/TD		

	IN CLASS HOURS	ECTS
SEMESTRE 2	188,5	30
BCC - IMPLEMENTING FUNDAMENTAL PHYSICS TOOLS AND APPROACHES TO PRODUCE HIGHLY SPECIALISED KNOWLEDGE	100	12
UE ELECTIVE COURSE UNITS (PICK 2 OUT OF 3 AMONG SCIENTIFIC PROGRAMMING, COMPUTATIONAL CHEMISTRY AND SPECTROSCOPIC IMAGING)	49	6
SB - Scientific Programming	24	3
EC - Scientific Programming 12h CM/TD - 12h TP		
SB - Computational Chemistry	24	3
EC - Computational Chemistry ¹ 12h CM/TD - 12h TP		
SB - Spectroscopic Imaging	25	3
EC - Spectroscopic Imaging 21h CM/TD - 4h TP		
UE - Large scale research infrastructures	27	3
EC - Large scale facilities in Physics - 20h CM/TD – 4h TD - 3h TP		
UE - Experimental project	24	3
EC - Experimental project 24h TP		
BCC - PRODUCING AND COMMUNICATING HIGHLY SPECIALIZED KNOWLEDGE, INCLUDING IN A PROFESSIONAL CONTEXT	16,5	9
UE - Internship	N/A	6
EC - Internship 0h TD		
UE - Tutored trainings	16,5	3
EC - Tutored trainings 4,5h CM/TD - 6h TD - 6h TP		
EC - Tutored trainings - Suivi 0h TD		
BCC - SOLVING COMPLEX PROBLEMS BY APPLYING FUNDAMENTAL PHYSICS CONCEPTS	72	9
UE - Condensed Matter 2	24	3
EC - Condensed matter II - Phonons 24h CM/TD		
UE - Fundamentals of molecular spectroscopy	24	3

EC - Fundamentals of molecular spectroscopy 24h CM/TD		
UE - Microstructures and defects in materials	24	3
EC - Microstructures and defects in materials 24h CM/TD		

TOTAL IN CLASS HOURS : 443H30

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 1

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 1

- **UE - States of Matter and Materials Science Primers** – 3 ECTS
 - *States of Matter and Materials Science Primers*
- **UE - Introduction to Pharmaceutical Materials Science** – 6 ECTS
 - *Introduction to Pharmaceutical Materials Science*
- **UE - Drug product development and pharmaceutical technology I** – 3 ECTS
 - *Drug product development and pharmaceutical technology I*

SEMESTRE 2

- **UE - Elective course units**– 6 ECTS
 - *Scientific Programming*
 - *Computational Chemistry 1*
 - *Spectroscopic Imaging*
- **UE - Large scale research infrastructures** – 3 ECTS
 - *Large scale facilities in Physics*
- **UE - Experimental project** – 3 ECTS
 - *Experimental project*

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 1

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 1

- **UE - Foreign language (1 choix) – 3 ECTS**
 - *FLE/FOU*
 - *Anglais*
- **UE - GP : Materials for a sustainable future – 3 ECTS**
 - *Materials for a sustainable future*
- **UE - Tutored trainings – 3 ECTS**
 - *Tutored trainings*

SEMESTRE 2

- **UE - Internship – 6 ECTS**
 - *Internship*
- **UE - Tutored trainings – 3 ECTS**
 - *Tutored trainings*

Grading rule for this BCC :

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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 1

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 1

- **UE - Continuum mechanics** – 3 ECTS
 - *Continuum mechanics*
- **UE - AI and advanced computational methods in physics** – 3 ECTS
 - *AI and advanced computations*
- **UE - Atomic scale modeling I – Classical methods** – 3 ECTS
 - *Atomic scale modeling I – Classical methods*
- **UE - Remediation**
 - *Remediation*

SEMESTRE 2

- **UE - Condensed matters II** – 3 ECTS
 - *Condensed matters II - Phonons*
- **UE - Fundamentals of molecular spectroscopy** – 3 ECTS
 - *Fundamentals of molecular spectroscopy*
- **UE - Microstructures and defects in materials** – 3 ECTS
 - *Microstructures and defects in materials*

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

SEMESTRE 1

STATES OF MATTER AND MATERIALS SCIENCE PRIMERS

UE : STATES OF MATTER AND MATERIALS SCIENCE PRIMERS

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

Class: mandatory

Teaching method: in person

Teaching language: English

Person in charge : Tiana Deplancke, tiana.deplancke@univ-lille.fr

Teaching team : Tiana Deplancke, Franck Beclin

Required prior teaching unit(s):

Suggested readings:

Syllabus :

Have a clear understanding of the different families of materials (metals and alloys, ceramics, polymers) based on their properties and microstructure.

Objectives :

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.

Outline:

- Generalities : the state of matter, crystalline and amorphous materials, Phenomenological approach of the diffusion process in gas and solid.
- Introduction to material science : Chemical bonding and the resulting physical and mechanical properties. Ashby diagram and main classes of materials.
- Ceramics: Introduction, properties and applications, diffusion process and elaboration process (sintering ...)
- Metals and alloys : Definition and structure, Phase diagram, phase transformation and microstructure resulting. Study case : Steel and iron carbon diagram.
- Polymers : Definition, macromolecular conformation, viscosity, classification of polymers, phenomenological and thermodynamical approaches of the glass transition, nucleation and growth of crystals, melting behavior.

Skills acquired:

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).

Evaluation methods

Continuous monitoring (1/2)

Final exam (1/2)

A solution will be offered for justified absences.

INTRODUCTION TO PHARMACEUTICAL MATERIALS SCIENCE

UE : INTRODUCTION TO PHARMACEUTICAL MATERIALS SCIENCE

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

Class: mandatory

Teaching method: in person

Teaching language: English

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

Teaching team : Emeline Dudognon, Natalia Correia, Frédéric Affouard

Required prior teaching unit(s):

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Suggested readings:

Syllabus :

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.

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.

i) Basic elements and interactions.

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. Interactions: ionic forces, hydrogen bonding, van der Waals, metallic, ionic and covalent bonds. Major classes of molecules and specificities (carbohydrates, polymers, biopolymers,...)

ii) Structure

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.

iii) Thermodynamics.

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.

The lectures are complemented by a 4-hour lab practical session on Differential Scanning Calorimetry (DSC) and X-ray diffraction techniques, focusing on the exploration of physical states (crystalline vs. amorphous) and their transformations, including melting, crystallization, and vitrification.

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

- Know the basic elements (atoms, ions, molecules) of materials and their interactions.
- Have general knowledge of the structure and microstructure of different states of matter.
- Have a basic understanding of the main structural and thermodynamical experimental characterization methods.
- Understand and analyse scientific reports concerning experimental studies concerning structure and thermodynamics of ordered and disordered condensed matter systems

Evaluation methods

1st session : final written exam, 3h

2nd session : oral exam

A solution will be offered for justified absences.

DRUG PRODUCT DEVELOPMENT AND PHARMACEUTICAL TECHNOLOGY I

UE : DRUG PRODUCT DEVELOPMENT AND PHARMACEUTICAL TECHNOLOGY I

BCC : IMPLEMENTING FUNDAMENTAL PHYSICS TOOLS AND APPROACHES TO PRODUCE
HIGHLY SPECIALISED 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):
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Suggested readings:

Syllabus :

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.

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.

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.

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 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:

- Have knowledge of the how a drug substance can be administered to a patient
- Be familiar with the most important pharmaceutical dosage forms (e.g. tablets, capsules, pellets, ointments, creams).
- Have knowledge of pharmaceutical materials, in particular excipients and their specificities
- Know the main approaches used for the manufacturing and quality control of drug products
- 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%)

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

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 methods

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 : Lucile Roberts lucile.roberts@univ-lille.fr

Required prior teaching unit(s):
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Suggested readings:

Syllabus :

■ ...

Evaluation methods

Continuous assessment:

- Listening comprehension 20%
- Speaking 30%
- Reading comprehension + language exercises 50%

Resit: oral exam

MATERIALS FOR A SUSTAINABLE FUTURE

UE : GP : MATERIALS FOR A SUSTAINABLE FUTURE

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

Class: mandatory

Teaching method: in person

Teaching language: English

Person in charge :

Sylvie Daviero-Minaud sylvie.daviero@univ-lille.fr

Grégory Stoclet gregory.stoclet@univ-lille.fr

Required prior teaching unit(s):
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Suggested readings:

Syllabus :

This PG Materials UE is an interdisciplinary course linked to various ULille master's programs in fields like chemistry, physics, mechanical engineering, and civil engineering, all focusing on materials for sustainable development. It aims to give master's students an overview of sustainable and multifunctional materials for various uses, such as energy, healthcare, textiles, and the environment. It also provides a framework for responsible research practices, useful in both academic and industrial settings. Additionally, it introduces the main challenges and tools of responsible research, focusing on scientific integrity, research ethics, data management and security, and open science.

The following are planned for the training semester:

- 4 seminars, each one hour long, on topics related to the PG.

These seminars are mandatory for all PG master's students, and attendance will be tracked. They will be recorded and available on the Moodle platform for students in work-study programs or apprenticeships to access remotely. After these seminars, a questionnaire will be posted and graded on Moodle.

- A half-day focused on the PG "Materials for a Sustainable Future," where various PG topics will be explained, along with an introduction to pursuing a doctorate or a research career. (Attendance will be checked)

In-person modules: These are designed to give master's students a framework for responsible research and lab practices. These modules will be assessed through online questionnaires (at least 3 are planned).

The specific goals of these modules are to:

- Make master's students aware of scientific integrity and research responsibilities. (Instructor: Éric Marceau)

- Make them aware of issues related to data management: protection, openness, and confidentiality. (*Instructors: Monica Michel Rodriguez and Tilila Lanux*)
- **Provide them tools for scientific communication, article writing, and introduce them to digital resources useful in research (bibliographic research tools, patent databases, etc.).** (*Instructor: Sébastien Merkel*)

Practical **case studies** will be provided through **guided discussions on “scientific integrity” and “Good data management: protection, openness and confidentiality”** and round tables on **“materials and society.”** These sessions aim to expose students to real-life situations, encouraging critical thinking, reasoned debate, and perspective on scientific, societal, and integrity-related issues in their field. The goal is to develop a broader understanding of the responsibilities linked to research activities.

Evaluation methods

Assessment: continuous assessment

- attendance check at lectures (attendance mandatory)
- online assessments (Moodle questionnaires) on the different parts of the UE (3 ECTS total, with a minimum of 3 questionnaires distributed over the semester)

TUTORED TRAININGS

UE : TUTORED TRAININGS

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

Class: mandatory

Teaching method: in person

Teaching language: English/French

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

Required prior teaching unit(s):
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Suggested readings:

Syllabus :
Discovery of new topics in physics based on the scientific literature and develop your teaching and presentation skills in front of your peers. Objectives 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) Course outline 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. In person activities: • Class 1 (1h30 CTD) Introduction, choice of subject, expectations • Class 2 (1h30 TD, 3 groups QPT, PMM, A2PM/BIOPHAM): Mid-course presentation, 10 minutes per pair, plan • Class 3 (1h30 TD, 3 groups) Presentation analysis session (based on students reports on the presentations of others, and on their own) • Class 4 (1h30 CTD) Latex and overleaf • Class 5 (1h30 CTD) Report preparation • Class 6 (1h30 TD, 3 groups) Final oral Tutor activities • propose a lead for topic (title, keywords, and references) • 3 individual meetings with the student pair they supervise • First contacts, first publications • Assessment of students' individual research and understanding of the topic

- Detailed plan of report
- Proofreading and evaluation of reports
- Participation in evaluation of oral defenses

Acquired skills

Develop advanced and critical expertise at the edge of knowledge in a sub-field of physics based on documents from the recent scientific literature

Identify, select, and critically analyze specialized resources to document a topic and make a synthesis and exploit their content

Present advanced scientific content in front of your peers

Evaluation methods

Report (1/3)

Oral defense (1/3)

Response to questions (1/3)

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

CONTINUUM MECHANICS

UE : CONTINUUM MECHANICS

BCC : SOLVING COMPLEX PROBLEMS BY APPLYING FUNDAMENTAL PHYSICS CONCEPTS

Class: mandatory

Teaching method: in person

Teaching language: English/French

Person in charge : *Philippe Carrez* – philippe.carrez@univ-lille.fr

Teaching team :

Required prior teaching unit(s):

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Suggested readings:

Syllabus :

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.

Requires

- Basis of linear algebra and crystallography

Objectives :

- acquire the basic concepts of continuum mechanics
- Define and manipulate stress and strain tensor, apply tensor transformation
- Analytically solve simple problems of elasticity

Course outline

- Stress and strain as a second-rank tensor
- Fundamental equations of elasticity, Hooke's law
- Navier equations
- Review of macroscopic plastic behavior of matter
- Principles stresses and yield criterion

Skills acquired

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.

Evaluation methods

1 final written exam, 2h

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.

AI AND ADVANCED COMPUTATIONS

UE : AI AND ADVANCED COMPUTATIONAL METHODS IN PHYSICS

BCC : SOLVING COMPLEX PROBLEMS BY APPLYING FUNDAMENTAL PHYSICS CONCEPTS

Class: mandatory

Teaching method: in person

Teaching language: English/French

Person in charge : *Quentin Coopman* – quentin.coopman@univ-lille.fr

Required prior teaching unit(s):

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Suggested readings:

- Thuerey, N., Holzschuh, B., Holl, P., Kohl, G., Lino, M., Liu, Q., Schnell, P., & Trost, F. (2021). **Physics-based Deep Learning**. <https://doi.org/10.48550/arxiv.2109.05237>
- Fidle CNRS : <https://www.fidle.cnrs.fr/>

Syllabus :

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.

Objectives :

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.

Course outline

- Courses (10H):
 - I - Introduction to Artificial Intelligence and Machine Learning (1H)
 - Overview of AI and ML
 - Applications in physics
 - Key concepts and terminology
 - II - Fundamentals of Machine Learning (1H)
 - Supervised vs. unsupervised learning
 - Regression, classification, prediction
 - Evaluation metrics
 - III - Classification/Clustering algorithms (1H30)
 - Linear Models and Regularization (Linear regression)
 - Decision Trees and Ensemble Methods (Decision trees, Random, Gradient boosting regression tree forests)
 - K-means
 - IV - Dimensionality reduction (e.g., Principal Component Analysis) (45 mins)

- V - Neural Networks and Deep Learning (2H15)
 - Introduction to neural networks
 - Activation functions
 - Training neural networks
 - Encodeur/Decodeur
- VI - Data Preprocessing (1H)
 - Handling physics data
 - Feature selection and extraction
 - Data normalization and scaling
 - Datacentric methods
- VII - Introduction Advanced Topics in Machine Learning for Physics (2H)
 - Physics-informed machine learning
 - Interpretable AI models
- Practicals (15H):
 - The practical sessions (TDs/TPs) will be conducted with the assistance of the CRI and the MesoNET program to access the notebooks. 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

- Grasp the fundamental principles of artificial intelligence and machine learning.
- Learn key terminology and concepts used in AI and ML.
- Apply AI and ML techniques to solve problems in the field of physics.
- Differentiate between and apply supervised and unsupervised learning techniques.
- Implement regression, classification, and prediction models.
- Use popular ML libraries and tools such as TensorFlow, PyTorch, and scikit-learn.
- Implement AI and ML techniques in practical, hands-on projects and case studies.
- Use advanced digital tools autonomously for one or more professions or research sectors in the field.
- 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.
- Develop predictive tools based on validated models describing complex physical problems.

Program digital tools to process physical measurements in a relevant manner (potentially using machine learning and AI approaches).

Evaluation methods

Continuous assessment and project

The course evaluation will consist of two main parts:

Multiple Choice Quiz at the beginning of some lectures (30%)

Project leading to a written report of analysis and interpretation of a dataset (70%)

ATOMIC SCALE MODELING I – CLASSICAL METHODS

UE : ATOMIC SCALE MODELING I – CLASSICAL METHODS

BCC : SOLVING COMPLEX PROBLEMS BY APPLYING FUNDAMENTAL PHYSICS CONCEPTS

Class: mandatory

Teaching method: in person

Teaching language: English/French

Person in charge : Céline Toubin – celine.toubin@univ-lille.fr

Teaching team : Frederic Affouard, Philippe Carrez, Céline Toubin

Required prior teaching unit(s):

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Suggested readings:

Syllabus :

Discover powerful simulation techniques like Molecular Dynamics to predict and design material properties at the atomic scale.

Objectives :

- Identify when and why to use atomistic simulations in research and development.
- Apply optimization techniques to obtain stable atomic or molecular structures.
- Set up and adapt force-field models for different material systems.
- Analyze simulation outputs using relevant physical and statistical quantities.

Course outline

- Why performing simulations?
- Optimization Techniques
- Force-field description
- Molecular dynamics principles: forces evaluation and cut off, periodic boundary conditions, minimum image convention, thermostat, barostat, statistical averages and observables
- Hands on practicals

Skills acquired

- **Optimize atomic structures** using energy minimization and relaxation techniques.
- **Identify appropriate simulation methods** for solving material and molecular-scale problems.
- **Understand and evaluate force-field models** for specific systems to achieve reliable predictive accuracy.
- **Implement key MD concepts**, including thermostats, barostats, cutoffs, and periodic boundary conditions.
- **Apply statistical mechanics principles** to extract thermodynamic and structural observables from simulation data.

Evaluation methods
Report and oral presentation A solution will be offered for justified absences or delays with the report or defense.

REMEDIATION

UE : REMEDIATION

BCC : SOLVING COMPLEX PROBLEMS BY APPLYING FUNDAMENTAL PHYSICS CONCEPTS

Class: mandatory

Teaching method: in person

Teaching language: English/French

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

Required prior teaching unit(s):

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Suggested readings:

Syllabus :

This is aimed to provide teaching hours for students who did not study in Lille and may need additional classes as they join the training in S1 or S3.

Program of the class will be adjusted as needed. According to experience in previous years, we may provide support on

- navigating operating systems and a basic computer environment,
- elements of computer programming,
- quantum mechanics,
- elasticity of materials.
- Other topics will be added, as required to assist our students.

There are no credit associated with this unit which is aimed at improving the success rate of our students.

Evaluation methods

None

SEMESTRE 2

SCIENTIFIC PROGRAMMING

UE : ELECTIVE COURSE UNITS

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

Class: mandatory

Teaching method: in person

Teaching language: English

Person in charge : *Silvio Pipolo* – silvio.pipolo@univ-lille.fr

Required prior teaching unit(s): basics of computing principles, hardware, software, operating system

Suggested readings : <https://www.python.org/about/gettingstarted/>

Syllabus :

- The first part of the course (10 hours) aims at setting the basis for the design of algorithms for simple programs. The basic concepts treated are listed below.
 - The bash terminal and basic instructions: listing files, creating and exploring directories, running programs etc.
 - Flowcharts and basic instructions: I/O, processes, decisions.
 - Logical connectors.
 - Loops, counters and accumulators.
- The second part of the course (18 hours) is devoted to the application of the concepts acquired in the first part to the writing and execution of python scripts and programs. Below a list of key concepts.
 - Variables, expressions and statements.
 - Strings, lists, dictionaries and indexes.
 - Principles of object programming.
 - Functions and classes.
 - File management.
 - Libraries for the management of matrices and tables (e.g. NumPy).
 - Techniques for data visualization and data analysis (the pandas library).
- The third part of the course (8 hours) is devoted to the application of the programming skills acquired to scientific case studies. The subject may change from year to year to match the needing of other teaching units!.

Evaluation methods

Report on practicals: 100%

Second session : Report on practicals: 100%

COMPUTATIONAL CHEMISTRY 1

UE : ELECTIVE COURSE UNITS

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

Class: mandatory

Teaching method: in person

Teaching language: English

Person in charge : *Florent Louis* – florent.louis@univ-lille.fr

Required prior teaching unit(s): Lectures conseillées :

Suggested readings :

Syllabus :

Description:

The main objective of the « Computational chemistry 1 » course is to confer solid background concerning the use of theoretical calculations that are being extensively used in our laboratories. This class is a compulsory prerequisite for "Computational chemistry 2" (S3).

Objectives:

The student will be able to understand basic knowledge of computational chemistry (methods, basis sets) and how to use them for obtaining molecular properties of interest.

From the computational point of view, the students will be able to manage a theoretical calculation from input to output files in order to optimize molecular geometry of fundamental states and transition states.

Program:

The computational chemistry classes will be divided in half fundamental lectures and half laboratory work. After an introduction to molecular modeling, the lectures will bring basic knowledge on the following topics: (1) molecular mechanics, (2) Hartree-Fock method, (3) Basis sets, (4) Molecular Properties, (5) Electron correlation, (6) Convergence of calculations. The labworks will be performed in computer rooms. They will allow students to be initiated to the use of Unix language. Several labworks will be done, covering the determination of: structural parameters (geometry and vibrational frequencies); infrared spectra; thermochemical properties for a species and a reaction; reaction intermediates (transition states, molecular complexes); and reaction mechanisms.

Evaluation methods

The final grade N will consist of 2 grades :

- One continuous assessment grade CC (50% of the final grade) based on the evaluation of labwork reports.
- One final grade CT (50% of the final grade) based on a written exam of 2h.

$N = 50\% \text{ CC} + 50\% \text{ CT}$

Second session : written exam, 2h, 50% ; the grade of continuous assessment is conserved, 50%

SPECTROSCOPIC IMAGING

UE : ELECTIVE COURSE UNITS

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

Class: mandatory

Teaching method: in person

Teaching language: English

Person in charge : Marie Choel – marie.choel@univ-lille.fr

Required prior teaching unit(s): atomic structure, light-matter interactions

Suggested readings :

- Murphy, D. B., & Davidson, M. W. (2012). Fundamentals of Light Microscopy and Electronic Imaging (2nd Edition). Wiley-Blackwell.

Syllabus :

- **Spectroscopic Imaging** is a multidisciplinary course aiming at providing a solid understanding of the principles behind microscopic and spectroscopic imaging. Learning outcomes include: preparing samples for microscopy; operating various optical systems; acquiring and adjusting spectral data; performing mappings; and conducting basic image analysis in order to extract chemical, structural, and spatial information from samples.
- Course contents:
 - Introduction: elements of optics (resolution, diffraction limit, aberration, microscope anatomy)
 - Principles and applications of:
 - transmission microscopy (a quick tour of an optical microscope)
 - fluorescence microscopy (sources, mirrors, filters)
 - confocal microscopy (scanning, sampling, multidimensional imaging)
 - Raman microscopy (excitation laser, diffraction grating, lateral and axial resolution)
 - FTIR microscopy (transmission, reflection and ATR modes)
 - Complementary microscopy techniques (elemental X-ray mapping by SEM/EDX, topographic and phase contrast imaging in AFM)
 - Practical case studies: visualization, analysis, quantification using ImageJ

Modalités d'évaluation

Online and written tests at the end of tutorial sessions (50%) + oral presentation (50%)

Oral 100%

LARGE SCALE FACILITIES IN PHYSICS

UE : LARGE SCALE RESEARCH INFRASTRUCTURES

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

Class: mandatory

Teaching method: in person

Teaching language: English/French

Person in charge : Manuel Goubet – manuel.goubet@univ-lille.fr

Teaching team : Eleonore Roussel eleonore.roussel@univ-lille.fr, Jean-François Brun jfbrun@univ-lille.fr,
Suzanne Crumeyrolle suzanne.crumeyrolle@univ-lille.fr, Andre Gomes andre.gomes@univ-lille.fr, Laurent
Margulès laurent.margules@univ-lille.fr

Required prior teaching unit(s):

Suggested readings:

Syllabus :

Objectives

This course aims to introduce students to the principles, functioning, and applications of major large scale research infrastructures (LSRI) used in both fundamental and applied research. It also seeks to develop cross-disciplinary skills such as literature review, critical analysis, and scientific communication.

Course outline

- General Introduction (2h)
Importance of LSRI, historical perspective, functioning, and scientific challenges
- Examples of scientific advancements thanks to LSRI (4.5h)
The Higg's boson
Gravitational waves
Event horizon of M87 black hole
- Case Study 1: Synchrotron Radiation (4.5h)
Working principles and applications
Introduction to coherent light sources (CLS)
- Case Study 2: Neutron Sources (2h)
Working principles and applications
Examples of performed researches
- Case Study 3: ACTRIS: Aerosol, Clouds and Trace Gases Research Infrastructure (3h)
Working principles and applications
Examples of performed researches
- Case Study 4: Millimeter/Submillimeter Astrophysics (3h)
Principles and significance of radio telescopes
Overview of major observatories: ALMA, GBT and NOEMA
Role in detecting prebiotic species and understanding the origins of life

- Case Study 5: Large Intensive Computing Equipment (2h)
Working principles, applications in physics, chemistry, and biology
Overview of major French facilities: CINES, IDRIS and TGCC
Examples of performed researches
- Visit of a research infrastructure (3h)
- Bibliographic review of a research article based on LSRI (4h)

Acquired skills

- Understanding the physical concepts underlying modern scientific instrumentation
- Knowledge of how large scale research infrastructures operate
- Ability to identify and analyze fundamental physical phenomena
- Ability to analyze and interpret scientific literature
- Clear and concise written and oral scientific communication

Evaluation methods

40 % written exam

40 % oral presentation of bibliographic review

20 % written report of laboratory visit

A solution will be offered for justified absences or delays.

EXPERIMENTAL PROJECT

UE : EXPERIMENTAL PROJECT

BCC1 : METTRE EN ŒUVRE DES OUTILS ET DES DEMARCHES DE PHYSIQUE FONDAMENTALE
POUR PRODUIRE DES SAVOIRS HAUTEMENT SPECIALISES

Class: mandatory

Teaching method: in person

Teaching language: English/French

Person in charge : *Manuel Goubet* – manuel.goubet@univ-lille.fr

Teaching team : *Suzanne Crumeyrolle* suzanne.crumeyrolle@univ-lille.fr, *François Anquez* francois.anquez@univ-lille.fr, *Clément Evain* clement.evain@univ-lille.fr

Required prior teaching unit(s):

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Suggested readings:

Syllabus :

Objectives

This course aims to develop students' autonomy, scientific rigor, and technical skills through the realization of an experimental project in pairs. It involves applying theoretical knowledge acquired so far to solve a real-world problem.

Course outline

- Design and implementation of an experimental setup or technical study
- Development of measurement protocols
- Use of specialized software
- Use of instruments related to the project
- Critical analysis of results
- Writing of a scientific report and oral presentation of the work

Acquired skills

- Project management in a team setting
- Development of an experimental scientific approach
- Proficiency in digital and instrumental tools
- Critical analysis of experimental data
- Autonomy and initiative
- Bibliographic research and data synthesis
- Professional communication (written and oral)
- Teamwork and collaboration

Evaluation methods

33% CC (logbook, implication)

33% written report

33% oral presentation

A solution will be offered for justified absences or delays.

INTERNSHIP

UE : INTERNSHIP

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

Class: mandatory

Teaching method: in person

Teaching language: English/French

Person in charge :

Required prior teaching unit(s):

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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 Internship - Skills - <i>Theoretical Skills</i> • Understanding how the work in a professional environment, either in the private or public research environment - <i>Technical and Professional Skills</i> • 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 2 months will take place between May 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 methods
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.

TUTORED TRAININGS

UE : TUTORED TRAININGS

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

Class: mandatory

Teaching method: in person

Teaching language: English/French

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

Required prior teaching unit(s):
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Suggested readings:

Syllabus :
Discovery of new topics in physics based on the scientific literature and develop your teaching and presentation skills in front of your peers. Objectives 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) Course outline 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. In person activities: • Class 1 (1h30 CTD) Introduction, choice of subject, expectations • Class 2 (1h30 TD, 1 group): 3 minutes pitch on the topic of study • Class 3 (1h30 TD, 1 group): Presentation analysis session (based on students reports on the presentations of others, and on their own) • Class 4 (1h30 CTD) Report preparation • Class 5 (1h30 CTD) Poster preparation • Class 6 (3h00 TD) Poster session Tutor activities • propose a lead for topic (title, keywords, and references) • 3 individual meetings with the student pair they supervise • First contacts, first publications • Assessment of students' individual research and understanding of the topic

- Detailed plan of report
- Proofreading and evaluation of reports
- Participation in the poster session

Acquired skills

Develop advanced and critical expertise at the edge of knowledge in a sub-field of physics based on documents from the recent scientific literature

Identify, select, and critically analyze specialized resources to document a topic and make a synthesis and exploit their content

Present advanced scientific content in front of your peers

Evaluation methods

Report (1/3)

Poster (1/3)

Response to questions (1/3)

A solution will be offered for justified absences or delays.

CONDENSED MATTER II – PHONONS

UE : CONDENSED MATTER II

BCC : SOLVING COMPLEX PROBLEMS BY APPLYING FUNDAMENTAL PHYSICS CONCEPTS

Class: mandatory

Teaching method: in person

Teaching language: English/French

Person in charge : Yan Pennec – yan.pennec@univ-lille.fr

Required prior teaching unit(s):

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Suggested readings:

Syllabus :

This lecture explores the vibrational properties of crystalline solids, from lattice symmetries and phonon dispersion to thermodynamic behavior. It provides the fundamental tools to understand heat capacity, thermal transport, and the quantum nature of lattice vibrations in condensed matter systems.

Prerequisites

Condensed Matter I (S1), Statistical Physics (L3), Crystallography. Bravais Lattices / Reciprocal Lattices / Brillouin Zone / Sum Rule, Fourier Analysis

Objectives

This course provides a rigorous introduction to the vibrational properties of crystalline solids. It develops the theoretical framework for lattice dynamics using classical and quantum models. It explains phonon dispersion, density of states, and their influence on thermodynamic properties. It analyzes how phonons govern specific heat, thermal conductivity, and electron interactions. It lays the foundation for understanding thermal and vibrational phenomena in condensed matter physics.

Course outline

Chapter 2: Dynamics of the Crystal Lattice :

Introduction / Harmonic Approximation / Vibrations of a One-Dimensional Atomic Lattice / Extension to Two and Three Dimensions / Quantification of Vibrations: Phonons / Conclusion

Chapter 3: Crystal Lattice Dynamics II

Introduction / Density of States / Thermodynamic Properties / Einstein Model of Specific Heat / Debye Model of Specific Heat / Phonon Scattering and Thermal Conductivity

Chapter 4 : Phonon Transport / Anharmonic Effects / Thermal dilatation (Grüneisen coefficient).

Acquired skills

At the end of the course, students are able to acquire and analyze phonon dispersion relations derived from lattice dynamics in one, two, and three dimensions. They can interpret how phonons influence the

thermal and electronic properties of solids, including specific heat and thermal conductivity. They understand and apply the Debye and Einstein models to explain the temperature dependence of specific heat, and can evaluate the role of electron-phonon interactions in condensed matter systems. They are also proficient in using theoretical frameworks—such as the harmonic approximation and the Brillouin zone formalism—to model and interpret the vibrational behavior of crystalline solids.

Evaluation methods

1 final written exam, 2h

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.

FUNDAMENTALS OF MOLECULAR SPECTROSCOPY

UE : FUNDAMENTALS OF MOLECULAR SPECTROSCOPY

BCC : SOLVING COMPLEX PROBLEMS BY APPLYING FUNDAMENTAL PHYSICS CONCEPTS

Class: mandatory

Teaching method: in person

Teaching language: English/French

Person in charge : *Roman Motiyenko* – roman.motiyenko@univ-lille.fr

Required prior teaching unit(s): Quantum mechanics, Atomic Physics

Suggested readings:

- C. Banwell, *Fundamentals of Molecular Spectroscopy*
- P.R. Bunker, P. Jensen *Fundamentals of Molecular Symmetry*
- P. Bernath, *Spectra of Atoms and Molecules*

Syllabus :

Course Objectives : Students will gain a solid understanding of the quantum mechanical principles behind molecular spectroscopy, with emphasis on rotational and vibrational transitions and the role of symmetry in determining spectroscopic activity.

- Block 1: Foundations & Born-Oppenheimer Approximation
 - Session 1: Introduction to molecular spectroscopy
 - Spectroscopic domains (microwave, IR, Raman)
 - Energy level structure of molecules
 - Overview of the molecular Hamiltonian
 - Session 2: Born-Oppenheimer approximation
 - Separation of electronic, vibrational, and rotational motion
 - Potential energy surfaces and electronic states
- Block 2: Molecular Rotation
 - Session 3: Rigid rotor model – Diatomics
 - Quantum mechanics of rotation
 - Rotational energy levels
 - Session 4: Rotational spectra of linear and symmetric top molecules
 - Selection rules (qualitative)
 - Effects of molecular structure on spectra
 - Session 5: Non-rigid rotor and centrifugal distortion
 - Real molecule corrections
 - Examples and simple spectra

- Block 3: Molecular Vibration
 - Session 6: Harmonic oscillator and vibrational quantization
 - Vibrational energy levels
 - IR activity of diatomics
 - Session 7: Normal modes in polyatomic molecules
 - Cartesian vs internal coordinates
 - Normal mode classification
 - Session 8: Anharmonicity and rovibrational transitions
 - Overtones, hot bands
 - Introduction to vibration-rotation spectra
- Block 4: Molecular Symmetry & Group Theory
 - Session 9: Symmetry elements and operations
 - Point groups, molecular examples
 - Session 10: Representations and character tables
 - Reducible and irreducible representations
 - Application to molecular motions
 - Session 11: Vibrational mode classification using group theory
 - Normal mode symmetry
 - Prediction of IR and Raman activity
- Block 5: Spectral Intensities & Selection Rules
 - Session 12: Transition dipole moments and intensity
 - Time-dependent perturbation theory overview
 - Einstein coefficients
 - Session 13: Symmetry-based selection rules
 - Direct product and integral criterion
 - Rotational and vibrational transition probabilities
- Block 6: Applications & Interpretation
 - Session 14: Interpretation of rotational spectra
 - Case studies (e.g., HCl, CO)
 - Spectroscopic constants and molecular geometry
 - Session 15: Interpretation of vibrational spectra
 - IR and Raman of polyatomic molecules
 - Examples: CO₂, H₂O, NH₃, etc.
 - Session 16: Final review and problem-solving workshop
 - Mixed exercises and discussion
 - Clarification of key concepts

Evaluation methods*Final exam*

A solution will be offered for justified absences.

MICROSTRUCTURES AND DEFECTS IN MATERIALS

UE : MICROSTRUCTURES AND DEFECTS IN MATERIALS

BCC : SOLVING COMPLEX PROBLEMS BY APPLYING FUNDAMENTAL PHYSICS CONCEPTS

Class: mandatory

Teaching method: in person

Teaching language: English/French

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

Teaching team : F. Béclin, A. Néri, Ph. Carrez

Required prior teaching unit(s):

Suggested readings:

Syllabus :

Materials are made of grains, defects, and other microstructural elements. The arrangement microstructural elements control the physical properties of materials and are the object of intense research and analysis, both in academic research, to understand the fundamentals of materials's plasticity or the history of deformation in the Earth's mantle, but also in direct contact with day-to-day applications, from the making of a beer canister to the effect of radiations inside a nuclear reactor.

Objectives

This class will help students understand:

- how microstructures control material performance and properties,
- the methods used to characterize and model microstructural development,
- the underlying physical principles governing microstructural evolution in a material,
- the prediction of materials properties based on modeling and EBSD observations.

The class will include classical teaching as well as hands on experience with data and computer software.

Course outline

Part I : Microscopic scale (8 hours)

- Elements of materials microstructures: phases, grains, defects, grain boundaries
- Dislocations and defects
- Crystal growth

Part II : Polycrystal scale (8 hours)

- Representation of microstructures: Euler angles, orientation distribution function, pole figures and inverse pole figures,
- Observation in electron microscopy and EBSD
- Plastic deformation: Schmid factor, Taylor and Sachs bounds, numerical modeling methods

- Polycrystal mechanical properties

Part III : Hands on experience (8 hours)

- Microstructure visualization with MTeX
- Visco-plastic self consistent modeling
- Interpretation of EBSD observations

Evaluation methods

Table exam on part I.

Table exam on part II.

Report of data interpretation and microstructure modeling.

A solution will be offered for justified absences.



Campus Cité scientifique

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