PEOPLE'S DEMOCRATIC REPUBLIC OF ALGERIA

MINISTRY OF HIGHER EDUCATION

AND SCIENTIFIC RESEARCH

Compliance and Harmonization Framework

TRAINING PROGRAM OFFER

L.M.D. Academic Master's Degree

2025 – 2026

Field	Program	Specialization
Materials Science	Chemistry	MATERIALS CHEMISTRY

I – Semester Course Organization Sheet
(S1, S2 et S3)

Semester 1 :

Teaching Unit (TU)	Courses	WLH	Weekly Hours (WH)			Others	Coeff	Credits	Assessment Method	
	Title	15 Weeks	L	TUT	PW				Assessment	Exam
Core Teaching Unit (CTU) Code : CTU 1 Credits : 18 Coefficient : 9	Solid State Chemistry	67h30	3h00	1h30		82h30	3	6	33%	67%
	Solid Phase Diagrams	45h00	1h30	1h30		55h00	2	4	33%	67%
	Materials Processing Methods 1	45h00	1h30	1h30		55h00	2	4	33%	67%
	Materials Characterization Techniques 1	45h00	1h30	1h30		55h00	2	4	33%	67%
Methodology Teaching Unit (MTU) Code : MTU 1 Credits : 9 Coefficient : 5	Practical: Materials Processing Methods 1	22h30			1h30	27h30	1	2	50%	50%
	Practical: Materials Characterization 1	22h30			1h30	27h30	1	2	50%	50%
	Artificial Intelligence and Machine Learning 1	15h00			1h00	10h00	1	1	50%	50%
	Physicochemical Properties of Materials	45h00	1h30		1h30	55h00	2	4	50%	50%
Introductory Teaching Unit (ITU) Code : ITU 1 Credits : 2 Coefficient : 2	Nanoscience and Nanotechnology	22h30	1h30			02h30	1	1		100%
	Thermal Analysis Methods	22h30	1h30			02h30	1	1		100%
Interdisciplinary Teaching Unit Code : ITU 1 Credits : 1 Coefficient : 1	Durability, Aging, and Recycling of Materials	22h30	1h30			02h30	1	1		100%
Semester 1 Total		375h	13h30	6h00	5h30	375h	17	30		

(WLH): Weekly Lecture Hours ; (L): Lecture ; (TUT): Tutorial ; (PW): Practical Work

Semester 2 :

Teaching Unit (TU)	Courses	VHS	Weekly Hours (WH)			Others	Coeff	Credits	Assessment Method	
	Title	15 Weeks	L	TUT	PW				Assessment	Exam
Fundamental Teaching Unit (FTU) Code : FTU 2 Credits : 18 Coefficient : 9	Applied Electrochemistry for Materials	67h30	3h00	1h30		82h30	3	6	33%	67%
	Materials Processing Methods 2	45h00	1h30	1h30		55h00	2	4	33%	67%
	Functional Materials	45h00	1h30	1h30		55h00	2	4	33%	67%
	Materials Characterization Techniques 2	45h00	1h30	1h30		55h00	2	4	33%	67%
Methodology Teaching Unit (MTU) Code : MTU 2 Credits : 9 Coefficient : 5	Practical: Spectroscopic Methods	22h30			1h30	27h30	1	2	50%	50%
	Materials Modeling	22h30	1h30			27h30	1	2		100%
	Chemometrics, Statistical Data Analysis, and Experimental Design	45h00	1h30		1h30	55h00	2	4	50%	50%
	Artificial Intelligence and Machine Learning 2	15h00			1h00	10h00	1	1	50%	50%
Discovery Teaching Unit Code : DTU 2 Credits : 2 Coefficient : 2	Semiconductors and Technological Applications	22h30	1h30			02h30	1	1		100%
	Emerging Pollutant Materials	22h30	1h30			02h30	1	1		100%
Transversal Teaching Unit Code : TTU 2 Credits : 1 Coefficient : 1	Materials Selection	22h30	1h30			02h30	1	1		100%
Semester 2 Total		375h	15h00	6h00	4h00	375h	17	30		

II - Detailed Program by Course

(One detailed sheet per course)

Adapt the course and tutorial (TD) programs according to the weekly on-site contact hours (VHH on-site) and the weekly individual workload hours (VHH personal).

Detailed Course Program for Semester S1

Semester: 1

Teaching Unit : Fundamental

Course : Solid State Chemistry

Course Objectives

The objective of this course is to enable students to become familiar with the different classes of solid materials and their main fields of application. It also aims to provide the fundamental and essential knowledge required for the understanding and study of the properties of solid materials.

Recommended Prerequisites

Undergraduate (Bachelor's) program in Chemistry

Course Content

1. Introduction (Suggested duration: 2 weeks)

- Different types of bonding in solids (covalent, ionic, metallic, intermolecular)
- Amorphous, crystalline, and semi-crystalline solids
- General properties of solids and classification of solids
- Primary substitutional solid solutions
- Secondary or intermediate substitutional solid solutions
- Interstitial solid solutions
- Stoichiometric compounds

2. Point Defects in Stoichiometric Solids (Suggested duration: 3 weeks)

- Intrinsic defects
- Neutral and charged defects; effective charge
- Rules for writing defect reactions
- Thermodynamic necessity of defects and defect equilibrium
- Chemical potential of defects and the law of mass action; structural units
- Chemical potential and activity of electrons

3. Point Defects in Non-Stoichiometric Solids (Suggested duration: 2 weeks)

- Non-stoichiometric compounds
- Examples of non-stoichiometric oxides
- Minority defects

4. Substitutions in Solids: Doping (Suggested duration: 2 weeks)

- Substitution by an element of the same valence
- Substitution by a lower-valence cation
- Substitution by a higher-valence cation

5. Formation and Ionization Energies of Defects. Defects in Band Diagrams (Suggested duration: 2 weeks)

- Defect formation energy
- Defects in band diagrams

6. Diffusion in Oxides (Suggested duration: 2 weeks)

- Diffusion kinetics
- Dependence of the diffusion coefficient
- Relationship between mobility and diffusion coefficient
- Conductivity in oxides

References (Books, lecture notes, websites, etc.)

– J.-F. Marucco: Chimie des solides (EDP Sciences)
– L. Smart and E. Moore: Introduction à la chimie du solide (Masson)
– L. Smart and E. Moore: Solid State Chemistry: An Introduction (Chapman & Hall)
– R. West: Basic Solid-State Chemistry (Wiley)
– P. F. Weller: Solid State Chemistry and Physics
– Progress in Solid State Chemistry (Series), Editor: Harold Reiss

Semester: 1

Teaching Unit: Fundamental

Course: Solid Phase Diagrams

Course Objectives

This course enables students to understand the fundamentals of thermodynamics and formal kinetics as applied to material systems. It also aims to develop mastery of the different types of binary phase diagrams (solid solutions, eutectic, peritectic systems, etc.) and the rules governing their interpretation. Finally, it allows students to apply this knowledge to industrial cases, such as reading bronze phase diagrams and optimizing heat treatments.

Recommended Prerequisites

A solid background in chemical thermodynamics is recommended, along with knowledge of general chemistry and physical chemistry of solutions (ideal and real solutions: activity, activity coefficient), as well as basic concepts related to metallic alloys: solid solutions, intermediate compounds, and fundamental definitions of eutectic and peritectic points.

Course Content

1. General Concepts (2 weeks)

- Concept of phase equilibrium
- Phase rule (Gibbs' phase rule)
- Lever rule
- Deviations from equilibrium
- Uncertainties in phase diagrams
- Phase nomenclature

2. Types of Binary Phase Diagrams: Case of Perfect Diffusion in the Solid and Liquid States (5 weeks)

- Alloys forming unlimited solid solutions
- Alloys forming limited solid solutions
- Alloys forming eutectic systems
- Alloys forming eutectoid systems
- Alloys forming peritectic systems
- Alloys forming peritectoid systems
- Alloys forming intermediate phases
- Alloys exhibiting a miscibility gap in the liquid state
- General case of equilibrium phase diagrams

3. Practical Case of Imperfect Diffusion: What Happens to Equilibrium Diagrams? (3 weeks)

- Case of spindle-shaped (lens-shaped) diagrams
- Case of eutectic diagrams

4. Applications of Equilibrium Phase Diagrams (2 weeks)

- Introduction to industrial applications

- Use in metallurgy and heat treatments

5. Reading and Interpretation of the Bronze Phase Diagram (3 weeks)

- Identification of different transformations and intermediate phases
- Practical diagram for industrial annealing treatments
- Practical diagram for as-cast foundry alloys

<u>References</u> (Livres et polycopiés, sites internet, etc.) :

· *Michel Soustelle : Thermodynamique des matériaux – École des Mines de Saint-Étienne (EDP Sciences), DOI:10.51926/ISTE.9781784051549*

· *Michel Dupeux : Introduction à la science des matériaux – Presses Polytechniques et Universitaires Romandes (PPUR)*

· *Robert W. Balluffi, Samuel M. Allen, W. Craig Carter : Kinetics of Materials – Wiley*

· *Jean-Noel Pons, Michel Robineau : Thermodynamique et équilibres chimiques – Cours et exercices corrigés*

· *Geneviève M.L. Dumas, Roger I. Ben-Aim : L'indispensable sur les diagrammes de phases*

· *C. Moreau, J.-P. Payen : Thermodynamique chimique – exercices et problèmes corrigés*

· *Alain Gruger : Thermodynamique chimique – Travaux dirigés*

· *A. Choukchou-Braham, M. Amine Didi : Cinétique chimique et catalyse*

Semester: 1

Teaching Unit: Fundamental

Course: Materials Processing Methods 1

Course Objectives

This course enables students to describe the different aspects of processing mineral or hybrid organo-mineral systems. It also aims to present their physicochemical properties and applications in ceramics, thin films, and nanomaterials.

Recommended Prerequisites

A solid understanding of phase equilibrium thermodynamics, mass transfer, heat transfer, and fluid mechanics is recommended.

Course Content

1. **Introduction (1 week)**
2. **Solid-State Reactions: Ceramic Method (3 weeks)**

- Reactants
- Mixing / Grinding
- Heat treatment
- Sintering: Determination of sintering temperature
- Applications of the ceramic method
- Limitations of the ceramic method

3. **Solution-Based Reactions: "Soft Chemistry" Methods (4 weeks)**

- Co-precipitation of hydroxides
- Sol-gel method: Mineral growth from molecule to material, hybrid materials
- Example applications of hybrid materials
- Decomposition of mixed complexes: Pechini method

4. **Hydrothermal (Solvothermal) and Combustion Methods (3 weeks)**

- Definition
- Experimental setup
- Advantages of the methods
- Limitations of the methods

5. **Colloid Chemistry (4 weeks)**

- Importance of research on nanoparticles
- Principles of colloidal synthesis of nanoparticles
- Physical properties of nanoparticles
- Examples of applications

References (Books, Lecture Notes, Websites, etc.)

- *Éric Felder : Matériaux - de l'élaboration à l'utilisation des matériaux - caractéristiques, obtention, emplois – Collection Technosup, Éditeur Ellipses (2020)*
- *Jean-Marie Haussonne, James L. Barton, Paul Bowen, Claude Paul Carry : Céramiques et verres, Principes et techniques d'élaboration – Traité des matériaux, Vol. 16*
- *Jean-Jacques Rousseau et Alain Gibaud : Cristallographie géométrique et radiocristallographie*
- *Didier Rioux : Introduction à la cristallochimie, solide cristallise et empilements compacts*

Semester: 1

Teaching Unit: Core Teaching Unit (CTU)

Course : Materials Characterization Techniques 1

Course Objectives

This course enables students to describe various aspects of processing mineral or hybrid organo-mineral systems. It also aims to present their physicochemical properties and applications in ceramics, thin films, and nanomaterials.

Recommended Prerequisites

A solid understanding of phase equilibrium thermodynamics, mass transfer, heat transfer, and fluid mechanics is recommended.

Course Content

1. X-Ray Diffraction (XRD)

- Introduction
- Crystalline and amorphous states; interaction of X-rays with matter; X-ray production
- X-ray diffraction principles; conditions for diffraction
- X-ray diffraction techniques
- Powder diffraction
- Experimental aspects of powder X-ray diffraction (chambers, diffractometer; sample preparation; factors affecting peaks)
- Recording a powder diffraction diagram
- Recording conditions
- Data obtained
- Interpretation of a powder diffraction diagram
- Peak identification
- Diagram decomposition
- Line profile refinement
- Full profile refinement
- Lattice parameter determination
- Single-crystal methods:
- Laue method
- Rotating crystal method
- Weissenberg method (hk0 and hkl diagrams)
- Precession method

2. Global Chemical Analysis Techniques

- X-ray fluorescence spectrometry (XRF)
- Emission spectrometry
- Inductively coupled plasma optical emission spectrometry (ICP-OES)
- Spark discharge spectrometry (SDL)

- Spark spectrometry
- Laser ablation analysis
- Gas analyzers: O, N, C, and S determination
- Oxygen and nitrogen analysis
- Carbon and sulfur analysis

3. Local Chemical Analysis Techniques

- X-ray microanalysis
- Castaing microprobe (instrument dedicated to microanalysis)
- Microanalysis using scanning electron microscopy (SEM) and transmission electron microscopy (TEM)
- Wavelength-dispersive spectrometry (WDS) for microprobe
- Energy-dispersive spectrometry (EDS) for SEM and TEM

4. Surface Characterization Techniques

- Photoelectron spectroscopy (ESCA or XPS) and Auger electron spectroscopy (elemental and chemical analysis)
- Spark discharge spectrometry (SDL)
- Secondary ion mass spectrometry (SIMS)

References *(Livres et polycopiés, sites internet, etc.) :*

- *M. Van Meersche et J. Feneau-Dupont : Introduction à la Cristallographie et à la Chimie Structurale*
- *D. Schwarzenbach : Cristallographie – Presses polytechniques et universitaires romandes, 1993*
- *J. Protas : Diffraction des rayonnements – Dunod (Paris), 1999*
- *J. J. Rousseau : Cristallographie géométrique et radiocristallographie – Masson (Paris), 1995*
- *C. Hammond : The Basis of Crystallography and Diffraction*
- *J. W. Smith : Geometrical and Structural Crystallography*
- *R. Guinebretière : Diffraction des rayons X sur échantillons polycristallins*

Semester: 1

Teaching Unit: Methodology (TUM)

Course: Practical Work: Materials Processing Methods 1

Course Objectives

This practical module aims to introduce students to various laboratory methods for processing solid materials, including solid-state routes, soft chemistry methods (sol-gel, co-precipitation), dry methods, and hydrothermal techniques. Emphasis is placed on acquiring experimental skills and critically analyzing the obtained results.

Recommended Prerequisites

Basic knowledge of general chemistry, solution chemistry, and fundamental laboratory techniques is recommended.

Course Content

- **Practical Work: Solid-State Method**
- **Practical Work: Soft Chemistry Methods**
- **Co-precipitation**
- **Sol-gel**
- **Citrate method**
- **Nitrate method**

- Practical Work: Dry (Classical) Methods
- Practical Work: Ceramic Methods
- Practical Work: Hydrothermal Synthesis of Semiconductor Metal Oxides (TCO)
- Practical Work: Hydrothermal Synthesis of Zinc Oxide (ZnO) Nanopowders
- Practical Work: Sol-gel Synthesis of SnO_2
- Practical Work: Modified Sol-gel Synthesis of TiO_2 Powders
- Practical Work: Preparation of Organic/Inorganic Composite Material
- Practical Work: Hydrothermal Synthesis of Semiconductor Metal Oxides

Semester: 1

Teaching Unit: Methodology (TUM)

Course: Practical Work: Materials Characterization 1

Course Objectives

This practical module introduces students to common materials characterization techniques, including X-ray diffraction (XRD), X-ray fluorescence (XRF), IR and UV-Vis spectroscopy, thermal analysis (TGA/DSC), and the use of open-source software for structural analysis. The focus is on understanding the principles, interpreting results, and critically analyzing experimental data.

Recommended Prerequisites
Basic knowledge of general chemistry, crystallography, materials physics, and fundamental laboratory skills is recommended. Familiarity with scientific computing tools is also useful.

Note: The list of practical sessions below is indicative and may vary depending on the resources available at each institution.

Course Content
Structural Characterization of Synthesized Nanocomposites
1. X-Ray Diffraction (XRD)

- Determination of lattice parameters and (hkl) indices for Cu, Zn
- Characterization of clay and pillared clay samples by XRD
- Determination of lattice parameters and phases in Cu-Zn alloy

2. X-Ray Fluorescence (XRF)

- Determination of the chemical composition of an aluminum alloy
- Determination of cement composition (example: ACC M'sila cement)

3. Spectroscopy
- Preparation of an organic/inorganic composite material and IR spectral analysis
- Coupling UV-Vis spectroscopy with electrochemistry to analyze concentration changes during electrochemical reactions

4. Thermal analysis
- Characterization of clay and pillared clay samples by TGA/DSC
- Determination of porosity in mineral-matrix nanocomposites

Practical Work with Open-Source Software
1. Visualization of Crystal Structures with VESTA

- Read CIF (Crystallographic Information File)
- Visualize crystal lattice, planes (hkl), coordination polyhedra
- Calculate interatomic distances, angles, and unit cell volumes

Activities:

- Open multiple CIF files (NaCl, graphite, quartz...)
- Display planes (100), (110), (111)
- Represent coordination polyhedra
- Export annotated images

2. Interpretation of Simulated XRD Patterns

- Understand diffraction peaks
- Identify planes (hkl) corresponding to peaks
- Verify Bragg's law

Activities:

- Use simulated diffractograms (e.g., NaCl powder, graphite)
- Associate each peak with a crystal plane
- Verify angular positions obey Bragg's law

3. Structure Refinement with FullProf (Rietveld Method)

- Use FullProf to refine a structure from experimental data
- Obtain lattice parameters, fit quality (Rwp, χ^2)

Activities:

- Load experimental powder diffraction file
- Create the .pcr file with EdPCR
- Adjust lattice parameters, scale factor, peak width
- Interpret refinement results

4. Phase Identification from Unknown Diffractogram

- Identify an unknown phase from experimental data
- Use crystallographic databases (ICSD, COD)

Activities:

- Receive an unknown powder diffraction file
- Simulate candidate diffractograms with FullProf
- Compare peaks and find the best match
- Justify the phase identification

5. Influence of Crystal Structure on Diffraction Patterns

- Compare diffractograms of different crystal structures
- Understand the effect of symmetry and lattice type (cubic, tetragonal, hexagonal…)

Activities:

- Compare NaCl (cubic), graphite (hexagonal), rutile-TiO_2 (tetragonal)
- Simulate diffractograms from CIF files

Identify the effects of symmetry on peak intensity and positions

Common Resources for All Practical Sessions
Software: VESTA, FullProf Suite (EdPCR, WinPlotr), PowderCell (optional)
CIF Files: Available at https://www.crystallography.net/cod/
Experimental or Simulated Data: Provided by the instructor

Or this program

Semester: 1

Teaching Unit: Methodology (TUM)

Course: Practical Work: Materials Characterization 1 – Software-Based

Course Objectives

This practical module introduces students to the use of open-source software for structural characterization of materials. It covers crystal visualization, interpretation of diffraction patterns, structural refinement using the Rietveld method, and identification of unknown phases from experimental data.

Recommended Prerequisites

A basic understanding of crystallography, X-ray diffraction, and familiarity with scientific computing tools is recommended.

Note: The list of practical sessions is indicative and may vary depending on the resources available at each institution.

Course Content

1. **Visualization of Crystal Structures with VESTA**

- Read a CIF (Crystallographic Information File)
- Visualize the crystal lattice and crystallographic planes (hkl)
- Calculate interatomic distances, angles, and unit cell volumes

Activities:

- Open multiple CIF files (NaCl, graphite, quartz…)
- Display planes (100), (110), (111)
- Represent coordination polyhedra
- Export annotated images

2. Interpretation of Simulated XRD Patterns

- Understand diffraction peaks
- Identify planes (hkl) corresponding to peaks
- Verify Bragg's law

Activities:

- Use simulated diffractograms (e.g., NaCl powder, graphite)
- Associate each peak with a crystal plane
- Verify angular positions according to Bragg's law
- Software used: WinPlotr, VESTA

3. Structure Refinement with FullProf (Rietveld Method)

- Learn to use FullProf for refining a structure from experimental data
- Obtain lattice parameters and fit quality (Rwp, χ^2)

Activities:

- Load an experimental powder diffraction file
- Create the .pcr file using EdPCR

- Adjust parameters: scale factor, peak width
- Interpret the refinement results

4. Phase Identification from an Unknown Diffractogram

- Identify an unknown phase from experimental data
- Use diffraction databases (ICSD, COD)

Activities :

- Receive an unknown powder diffraction file
- Simulate candidate diffractograms using FullProf
- Compare peaks to find the best match
- Justify the phase identification

5. Influence of Crystal Structure on Diffraction Patterns

- Compare diffractograms of different crystal structures
- Understand the effect of symmetry and lattice type (cubic, tetragonal, hexagonal…)

Activities :

- Compare NaCl (cubic), graphite (hexagonal), rutile-TiO_2 (tetragonal)
- Simulate diffractograms from CIF files
- Identify effects of symmetry on peak intensity and positions

<u>Common Resources for All Practical Sessions</u>

- Software: VESTA, FullProf Suite (EdPCR, WinPlotr), PowderCell (optional)
- CIF Files: Available at https://www.crystallography.net/cod/
- Experimental or Simulated Data: Provided by the instructor

Semester: 1

Teaching Unit: Methodology (TUM)

Course: Artificial Intelligence and Machine Learning 1

Course Objectives

This course aims to provide students with the fundamentals of Artificial Intelligence (AI) and Machine Learning (ML), with a particular focus on applications in materials science. Students will learn the core concepts of data-driven modeling and how to apply machine learning techniques to solve practical problems related to material properties and structures.

Recommended Prerequisites

A basic knowledge of programming (especially Python), statistics, and chemistry or physics of materials is recommended.

Course Content

1. **Introduction to AI and Machine Learning (2 weeks)**
    - Overview of Artificial Intelligence and its application areas
    - Importance of data in AI and Machine Learning

2. **Basic Concepts of Machine Learning (3 weeks)**
    - Supervised vs. unsupervised learning
    - Key ML algorithms: regression, classification, clustering
    - Evaluation metrics (MAE, R^2, accuracy)

3. Data Collection and Processing (3 weeks)

- Feature engineering and data preprocessing techniques
- Handling overfitting and underfitting
- Materials databases: Materials Project, OQMD, AFLOW

4. Practical Machine Learning in Materials Science (3 weeks)

- Case study: predicting material properties (bandgap, etc.)
- Using ML models for simple classification and regression tasks

5. Fundamentals of Deep Learning (3 weeks)

- Introduction to neural networks
- Major deep learning frameworks: TensorFlow, Keras, PyTorch
- Application: predicting crystal structures using neural networks

References (Books, Handouts, Websites, etc.) :

- *Aurelien Geron : *Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow* – O'Reilly Media (2019)*
- *Christopher M. Bishop : *Pattern Recognition and Machine Learning* – Springer (2006)*
- *Langage de programmation : Python*
- *Environnements : Jupyter Notebooks*
- *Bibliothèques : Scikit-learn, Pandas, Matplotlib*
- *Outils dédiés aux matériaux : Matminer, Pymatgen*

Semester: 1

Teaching Unit: Methodology (TUM)

Course : Physicochemical Properties of Materials

Course Objectives

This course aims to develop an understanding and analysis of the physicochemical properties of materials, with particular emphasis on their dielectric, magnetic, elastic, mechanical, thermal, and optical behaviors. By the end of the semester, students will be able to identify, interpret, and correlate these properties with the atomic and microstructural characteristics of materials.

Recommended Prerequisites

To effectively follow this course, students should have a basic background in the structure of matter (crystalline structures, atomic bonding). An understanding of fundamental material properties (conductivity, stiffness, mechanical behavior under stress) is also recommended, along with basic knowledge of applied mathematics for modeling certain physical phenomena.

Course Content

1. From the Atom to the Material (6 weeks)

- Atoms – Bonding – Structure (crystalline and amorphous materials)
- Classification of materials: metals and alloys – ceramics and glasses – polymers
- Composite materials

2. Electrical Properties (6 weeks)

- Electrical conductivity
- Metals, insulators, and semiconductors

3. Magnetic Properties (8 weeks)

- Magnetic moment
- Diamagnetism, paramagnetism, ferromagnetism, antiferromagnetism, ferrimagnetism
- General aspects of the magnetostrictive effect
- Magnetoelectric coupling
- Applications

4. Optical Properties (6 weeks)

- Light absorption, reflection, and transmission
- Optical materials: semiconductors, glasses, polymers
- Applications: photovoltaics, optoelectronics

5. Thermal Properties (6 weeks)

- Thermal expansion
- Thermal conduction
- Thermal diffusion

References (Books, Handouts, Websites, etc.) :

· C. Kittel: Introduction to Solid State Physics – Wiley, (2005)
· Michel Soustelle : Aide-mémoire Science des Matériaux – Dunod, Paris, (2004) (pp. 89–130)
· W. D. Callister : Materials Science and Engineering: An Introduction – Wiley, (2007)
· A. Moliton : Physique des matériaux pour l'électronique* – Hermès-Lavoisier, (2007)

Semester: 1

Teaching Unit: Discovery (TUD)

Course: Nanoscience and Nanotechnology

Course Objectives

This course aims to introduce students to the fundamental principles of nanoscience and nanotechnology, as well as their wide range of applications in areas such as energy, healthcare, nanoelectronics, spintronics, and other advanced technological fields.

Recommended Prerequisites

Students are expected to have a solid background in materials science, along with basic knowledge of thin film fabrication techniques.

Course Content

1. Preamble: Current Context of Nanoscience and Nanotechnology

2. Introduction to Nanoscience (2 weeks)

- The nanoscale and its applications
- Matter behavior at the nanoscale
- Nanofabrication processes
- Definitions and application fields: a multidisciplinary perspective

3 Fabrication and Characterization Tools for Nano-Objects (3 weeks)

- Nano-object fabrication techniques: how to fabricate nanostructures, different approaches
- Observation techniques at the nanoscale: microscopy tools used for nanoscale characterization

4. Nanochemistry (3 weeks)

- Carbon-based nanomaterials and related nanostructures: application examples
- Nanoparticle synthesis (various strategies), porous solids

5. Nanophysics (3 weeks)

- Nanoelectronic components: quantum effects in electronic transport at the nanoscale, silicon-based nanoelectronics
- Nano-optical structures: light–matter interaction at the nanoscale, colors and nanoparticles, emission, guiding, and detection of light using nanocomponents

6. Nanobiotechnology (3 weeks)

- Nanobiology: observing living systems at the nanoscale, detecting molecular interactions, manipulating nanometric biological objects
- Nanomedicine: nanodrugs, nanocarriers, design of nanocarriers for targeted delivery, interactions with cells
- Micro- and nanofluidics: fluid flow laws at the micro/nanoscale, biomolecule characterization in nanopores, lab-on-a-chip systems, digital microfluidics

7. Nanoscience and Society (2 weeks)

- Nanoscience and science policy
- Nanotoxicology: health-related challenges and impacts of nanoparticles
- Ecotoxicology: environmental issues
- Regulations: regulatory framework of nanotechnologies

References *(Books, Handouts, Websites, etc.) :*

- *Luque, S. Hegedus: Handbook of Photovoltaic Science and Engineering – Wiley*
- *Marti : Next Generation Photovoltaics– Taylor & Francis Group*
- *Yves Quéré : Physique des matériaux – Ellipses*
- *Périodiques : Solar Energy Materials & Solar Cells, Applied Physics*

Semester: 1

Teaching Unit: Discovery (TUD)

Course: Thermal Analysis Methods

Course Objectives

Thermal analysis methods provide students with fundamental knowledge used in the characterization of synthesized materials. This course aims to introduce the principles, techniques, and applications of thermal analysis in materials science.

Recommended Prerequisites

Students are expected to have a solid background in thermal analysis, particularly an understanding of physicochemical phenomena associated with thermal variations.

Course Content

1. Thermal Analysis (3 weeks))

- General principles of thermal analysis methods
- Overview of thermal analysis techniques:
- Thermogravimetric Analysis (TGA)
- Differential Thermal Analysis (DTA)
- Differential Scanning Calorimetry (DSC)
- Combined TG–DSC analysis
- Instrumentation used in thermal analysis

2. Thermogravimetric Analysis (TGA) (4 weeks)

- Definition
- Principle
- Parameters obtained from TGA curves
- Applications of TGA
- Theoretical shape of a TGA curve
- Main factors affecting TGA curves
- Kinetic interpretation of a TGA curve
- Coupled Differential Thermal and Thermogravimetric Analysis

3. Dilatometry (3 weeks)

- Thermal dilatometry
- Differential dilatometry

References *(Books, Handouts, Websites, etc.):*

- *A-P Bouaziz, R Rollet : *L'Analyse Thermique* – Tome 2*
- *Robert F. Speyer : *Thermal Analysis of Materials**

Semester: 1

Teaching Unit: Transversal (TUT)

Course: Durability, Aging, and Recycling of Materials

Course Objectives

This course enables students to master the concept of material durability and to understand the mechanisms that can alter material structure while maintaining the functions for which the material was designed. By the end of the semester, students will be able to identify different types of aging, the parameters influencing durability, and their impact on the main families of materials.

Recommended Prerequisites

Students are expected to have a solid background in physicochemistry and materials physics. Required knowledge includes general chemistry, physical chemistry, analytical chemistry, as well as the fundamental properties of materials.

Course Content

1. Durability (3 weeks)

- Definition
- Objectives of durability assessment
- High-temperature durability
- Durability in humid environments

2. Aging (5 weeks)

- Definition of aging
- Principles of material aging
- Physical aging
- Chemical aging
- Biological aging
- Aging mechanisms
- Thermal aging
- Photochemical aging
- Hydrolytic aging of materials
- Aging due to solvent absorption and hydrolysis
- Aging by additive migration
- Natural aging
- Accelerated artificial aging
- Aging induced by ionizing radiation
- Methods for service life prediction

3. Sustainable Design (2 weeks)

4. Aging, Durability, and Risk Management (3 weeks)

References *(Books, Handouts, Websites, etc.) :*

- *OFTA : Observatoire Français Des Techniques Avancées, *Vieillissement et durabilité des matériaux*, Sciences & Techniques, 8 Juin 2003*

III - Detailed Course Syllabus by Subject – Semester S2

Semester: 2

Teaching Unit (TU): Fundamental

Course Title: Applied Electrochemistry of Materials

Course Objectives

This course aims to provide students with a solid understanding of the fundamentals of electrochemistry applied to materials. It also enables them to implement and analyze the main electrochemical techniques used for materials characterization and surface modification. By the end of the course, students will be able to design and plan experimental protocols adapted to applications such as energy storage, corrosion, and materials protection.

Recommended Prerequisites

Students are expected to have a good mastery of redox reactions and solution electrochemistry.

Course Content (15 weeks)

Chapter 1: Fundamentals of Applied Electrochemistry (3 weeks)

- Electrochemical thermodynamics:
- electrochemical reactions, Gibbs free energy of electrochemical reactions, electrochemical potential, electrochemical systems
- Types of electrodes
- Nernst equation
- Electrochemical double-layer models: Helmholtz, Gouy–Chapman, Stern
- Pourbaix diagrams
- Electrochemical kinetics:
- Electrode polarization (overpotential)
- Kinetic regimes:
- Charge transfer (Butler–Volmer equation)
- Pure diffusion (steady-state diffusion flux, concentration profiles)
- Mixed regime (activation/diffusion control)

Chapter 2: Classical and Advanced Electrochemical Methods (4 weeks)

- Electrochemical setups:
- Two-electrode system
- Three-electrode system (reference, auxiliary, and working electrodes)
- Potentiostat–galvanostat
- Voltammetric techniques:
- Linear sweep voltammetry under pure charge-transfer control and pure diffusion control
- Cyclic voltammetry applied to redox species in solution and to materials
- Pulse voltammetry (normal pulse, differential pulse, square-wave)
- Electrochemical titrations:
- Amperometric titration at constant potential
- Potentiometric titration at zero current
- Electrochemical impedance spectroscopy (EIS)
-

Chapter 3: Corrosion and Protection of Materials (4 weeks)

- Types and morphologies of aqueous corrosion
- Corrosion cell operation:
- Single-electrode case
- Two-electrode (galvanic) cell
- Corrosion investigation methods:
- Tafel method
- Linear polarization resistance method
- Evans diagrams
- Electrochemical impedance spectroscopy
- Corrosion rate measurements:
- Gravimetric methods (immersion, mass loss, thickness loss)
- Electrochemical methods (Faraday's first and second laws)
- Materials durability
- Protection methods:
- Natural protection (passivation)
- Physical protection (organic coatings: varnishes, paints, epoxy resins)
- Chemical protection (manganese and zinc phosphating)
- Metallic coatings:
- Hot-dip galvanizing
- Electroplating
- Metallic particle-based coatings
- Electrochemical protection:
- Cathodic protection (sacrificial anodes and impressed current systems)
- Anodic protection (anodization of Ti, stainless steels, Al, Cr)
- Electropolymerization
- Corrosion inhibitors:
- Classes of inhibitors
- Mechanisms of action
- Inhibition efficiency
- Industrial applications (e.g., oil and gas industry)

Chapter 4: Electrodeposition and Surface Modification (2 weeks)

- Deposition kinetics
- Overpotential and layer growth
- Metallic, alloy, and functional coatings
- Electrochemical surface treatments

Chapter 5: Electrochemistry and Photoelectrochemistry of Semiconductors (2 weeks)

- Electrochemistry of semiconductors
- Mott–Schottky relationship
- Photoelectrochemical reactions and photoelectrolysis
- Applications to hybrid materials

<u>References recommandées :</u>

- Fabien Miomandre, Electrochemistry: From Concepts to Applications
- Allen J. Bard & Larry R. Faulkner, Electrochemical Methods: Fundamentals and Applications
- D. Landolt, Corrosion and Surface Chemistry of Metals
- Robert Roux, Chemical and Electrochemical Thermodynamics
- Jean Besson, Thermodynamics and Electrochemical Kinetics
- Software tools: EC-Lab Viewer, ElChemAnalyzer, Python (SciPy, Matplotlib)

Semester: 2

Teaching Unit (UE): Fundamental

Course Title: Materials Processing Methods 2

Course Objectives

The objective of this course is to address the different stages involved in the fabrication of a nanostructure according to the targeted application and the required characterization techniques. It also aims to present the main methods for the processing of inorganic materials and nanostructures, as well as to introduce thin film and nanostructure preparation techniques.

Recommended Prerequisites

Students are expected to have solid background knowledge in nanoscience and nanotechnology, materials chemistry and physics, electrochemistry, and the physico-chemical properties of materials.

Course Content

1. Introduction and Processing Strategies (2 weeks)

2. Processing by Mechanochemical Methods (5 weeks)

- Mechanosynthesis (Mechanical Alloying)
- Amorphization by mechanosynthesis
- Nanocrystal formation by mechanosynthesis
- Parameters influencing the nature of the product obtained by mechanosynthesis:
- Milling time
- Materials of containers and balls
- Nature of the powder
- Nature of gases
- Microwave synthesis:
- Principle
- Equipment
- Applications

3. Single-Crystal Growth (6 weeks)

- Single-crystal growth from the molten state
- Czochralski method (pulling technique)
- Kyropoulos method
- Bridgman–Stockbarger method
- Verneuil method
- Vertical zone melting
- Single-crystal growth from solvents (solution crystallization)
- Flux method

4. Thin Film Processing (9 weeks)

- Introduction to thin films
- Importance and technological applications of thin films
- Kinetic theory of gases

- Vacuum techniques: generation and measurement
- Growth mechanisms and growth modes
- Different growth modes
- Characterization of growth modes
- Nucleation and crystal growth
- Organized growth
- Main thin film deposition techniques:
- Classification
- Chemical techniques: electrodeposition, chemical bath deposition, sol–gel, etc.
- Physical techniques: vacuum evaporation, sputtering, molecular beam epitaxy (MBE), laser ablation, etc. Caractérisation du mode de croissance

References *(Books, lecture notes, websites, etc.) :*
- Ceramics and Glasses: Principles and Processing Techniques – Treatise of Materials, Volume 16
- B. R. Pamplin: Crystal Growth
- J. C. Brinker, G. W. Scherer: Sol-Gel Science: The Physics and Chemistry of Sol/Gel Processing
- Zangwill: Physics at Surfaces – Cambridge University Press, 1988
- L. Feldman, J. W. Mayer: Fundamentals of Surface and Thin Film Analysis – PTR Prentice-Hall Inc., 1986
- M. Villain, A. Pimpinelli: Physics of Crystal Growth – Éditions Alea Saclay, 1995

Semester: 2

Teaching Unit (TU): Fundamental

Course: Functional Materials

Course Objectives

This course enables students to gain an in-depth understanding of materials whose physical and chemical properties lead to specific applications in fields such as electronics, energy, health, and the environment. Particular emphasis is placed on the relationship between structure, properties, and functionality.

Recommended Prerequisites

A solid background in general chemistry, materials physics, basic concepts of crystallography, and the fundamental principles of thermodynamics and electrical properties of materials is recommended.

Course Content

1. Introduction to Functional Materials (2 weeks)

- Definitions and classification
- Difference between structural materials and functional materials
- Application areas (electronics, optics, magnetism, energy, sensors, etc.)

2. Fundamental Physicochemical Properties (3 weeks)

- Electrical and thermal conductivity
- Dielectric and ferroelectric properties
- Magnetic properties
- Thermoelectric, piezoelectric, and electrochemical effects

3. Conductive and Semiconducting Materials (4 weeks)

- Metals, alloys, and transparent conductive oxides
- Inorganic semiconductors (Si, GaAs, etc.)
- Organic semiconductors and conducting polymers
- Applications: diodes, transistors, photovoltaic cells

4. Materials for Optoelectronics (3 weeks)

- Light-emitting diodes (LEDs)
- Semiconductor lasers
- Phosphorescent and fluorescent materials

5. Materials for Energy Storage and Conversion (4 weeks)

- Fuel cells
- Batteries (Li-ion, Li–S, Na-ion, etc.)
- Supercapacitors
- Materials for electrocatalysis (HER, OER)

6. Magnetic Materials and Their Applications (4 weeks)

- Types of magnetism (ferro-, ferri-, antiferromagnetism, etc.)
- Soft and hard magnetic materials
- Applications: memory devices, sensors, spintronic devices

References (Books, Lecture Notes, Websites, etc.)

- William D. Callister, Materials Science and Engineering: An Introduction
- B. I. Sharma, Functional Materials: Preparation, Processing, and Applications
- A. S. Edelstein & R. C. Cammarata, Nanomaterials: Synthesis, Properties and Applications
- Collège de France lectures, online courses (OCW, MOOCs), and recent scientific articles (journals such as Advanced Materials, Nature Materials)

Semester: 2
Teaching Unit (TU): Fundamental
Course: Materials Characterization Methods 2

Course Objectives

This course enables students to understand the principles and applications of the major techniques used in the study and characterization of materials and nanostructures. It also aims to familiarize students with advanced spectroscopic and microscopic techniques for the structural, morphological, optical, and electrical analysis of materials.

Recommended Prerequisites

A solid background in nanoscience and nanotechnology, materials chemistry and physics, electrochemistry, as well as the physicochemical properties of materials is recommended.

Course Content

1. Introduction (1 week)

2. Scanning Probe Microscopy: Near-Field Microscopy (AFM, STM, etc.) (4 weeks)

- Presentation of nanoscale visualization techniques
- Scanning Tunneling Microscopy (STM)
- Atomic Force Microscopy (AFM)

3. Electron Beam Microscopy (SEM, TEM) and EDS Microanalysis (8 weeks)

- Operating principles of SEM: image formation and detection modes. X-ray microanalysis (EDS/EDX): principles and applications for local elemental analysis. Sample preparation for SEM.
- Operating principles of TEM: image formation and contrast modes (diffraction, mass–thickness contrast). Complementary techniques (electron diffraction, chemical analysis by Electron Energy Loss Spectroscopy, EELS). Sample preparation for TEM (thinning).
- High-resolution electron microscopy: use of apertures, contrast, and image interpretation.

4. Optical Characterization (Photoluminescence, Raman, Optical Band Gap) (5 weeks)

- Photoluminescence spectroscopy: principles and applications
- Raman spectroscopy: principles and applications
- Determination of the optical band gap from UV–Vis spectra

5. Electrical Characterization: Conductivity Measurement and Hall Effect (6 weeks)

- Electrical methods: electronic conductivity in powders, two-probe method
- Electronic conductivity in bulk samples: four-probe method. Ionic conductivity. Seebeck effect and Hall effect

References *(Books, Lecture Notes, Websites, etc.) :*

- Williams, D. B., & Carter, C. B. (2009). Transmission Electron Microscopy: A Textbook for Materials Science (2nd ed.). Springer
- Goldstein, J. et al. (2017). Scanning Electron Microscopy and X-Ray Microanalysis (4th ed.). Springer
- Cullity, B. D., & Stock, S. R. (2014). Elements of X-Ray Diffraction (3rd ed.). Pearson

Semester: 2

Teaching Unit (TU): Methodology

Course: Practical Work (Lab): Spectroscopic Methods

Course Objectives

The objective of this practical module is to train students in the use of the main physicochemical spectroscopic analysis methods. By the end of the semester, students will be able to perform qualitative and quantitative analyses using common spectroscopic techniques.

Recommended Prerequisites

It is recommended that students have acquired fundamental knowledge in analytical chemistry and materials characterization, as taught in fundamental teaching units at the undergraduate (Bachelor's) level.

Course Content

- Laboratory work on UV–Visible spectroscopy
- Laboratory work on IR spectroscopy
- Laboratory work on mass spectrometry
- Laboratory work on atomic absorption and emission spectroscopy
- Laboratory work on GC (Gas Chromatography) analysis
- Laboratory work on HPLC analysis
- Laboratory work on AAS or colorimetric analysis
- Laboratory work on other necessary characterization methods

References (Books, Lecture Notes, Websites, etc.)

- Maurice Pinta et al.: Atomic Absorption Spectrometry – Applications to Chemical Analysis, Masson et Cie, Paris, 1971
- Steve Gillet, D. Sc.: Course on Analytical Chemistry and Materials Characterization – Spectrometry – http://perso.latribu.com/shagar
- P. Rollet; R. Bouaziz: Thermal Analysis, Gauthier-Villars, Paris, 1972
- Douglas A. Skoog, Donald M. West, James J. Holler: Analytical Chemistry, De Boeck Editions, 1997

Semester: 2

Teaching Unit (TU): Methodology

Course: Materials Modeling

Course Objectives

This course enables students to appreciate the importance of constructing models that closely represent reality in order to extract meaningful information about the properties of the studied system. It also aims to familiarize students with the basic tools of molecular modeling and to enable them to interpret the underlying phenomena related to calculated observables and physical quantities.

Recommended Prerequisites

Students are recommended to have a solid understanding of the undergraduate curriculum in theoretical chemistry and the fundamentals of materials physics.

Course Content

1. **Fundamentals of Quantum Mechanics Applied to Materials (4 weeks)**

- Fundamental principles: wave function, Hamiltonian, Schrödinger equation
- Hartree–Fock (HF) method, Density Functional Theory (DFT) – basic approximations

2. **Atomistic Modeling Methods (5 weeks)**

- Interatomic potentials: Lennard-Jones, Morse, Embedded Atom Method (EAM)
- Molecular dynamics: Verlet algorithm, thermostats (NVE, NVT, NPT)
- Monte Carlo methods and statistical sampling

3. **Mesoscopic Modeling Methods (4 weeks)**

- Mean-field methods
- Brownian dynamics
- Cellular automata and percolation methods

4. **Simulation of Electronic Properties (5 weeks)**

- Band structure, density of states (DOS)
- DFT calculations: VASP, Quantum ESPRESSO, etc.
- Electrical conductivity and doping effects

5. **Simulation of Mechanical and Thermal Properties (5 weeks)**

- Young's modulus, stress–strain behavior, fracture, dislocations, cracks
- Heat transport: Fourier law, phonons
- Heat capacity, thermal conductivity

6. **Modeling of Interfaces and Surfaces (4 weeks)**

- Surface energy, adsorption, wetting
- Solid/liquid and solid/solid interfaces
- Simulation of thin films and atomic layers

References (Books, Lecture Notes, Websites, etc.)

Van Santen, Rutger A., Sautet, Philippe (Eds.): Computational Methods in Catalysis and Materials Science, Wiley, 2009

Feliciano Giustino: Materials Modelling Using Density Functional Theory: Properties and Predictions, Oxford University Press, 2014

Richard LeSar: Introduction to Computational Materials Science: Fundamentals to Applications, Cambridge University Press, 2014

Z. Xiao Guo (Ed.): Multiscale Materials Modelling: Fundamentals and Applications, CRC Press Inc., 2009

David Sholl, Janice A. Steckel: Density Functional Theory: A Practical Introduction, Wiley-Interscience, 2009

Semester: 2

Teaching Unit (TU): Methodology

Course: Chemometrics, Data Analysis, and Design of Experiments

Course Objectives

The main objective of this course is to train students in a rational and systematic approach to experimental problem-solving. By the end of the semester, students will be able to:

- *Understand the principles of chemometrics applied to experimental data*
- *Extract relevant and reliable information from complex and multivariate chemical data*
- *Master the statistical and mathematical tools required for efficient exploitation of experimental results*
- *Understand the different types of experimental designs and be able to choose or develop the most appropriate design to model and optimize a chemical system*

Recommended Prerequisites

Students are recommended to have a solid background in basic statistics, data analysis, and analytical chemistry.

Course Content

1. ***Fundamentals of Statistics Applied to Chemistry (3 weeks)***

- *Descriptive statistics: mean, median, variance, standard deviation, coefficient of variation*
- *Probability distributions: normal distribution, histograms, box plots*
- *Hypothesis testing: Student's t-test, chi-square test, one-way ANOVA*
- *Confidence intervals and significance level (p-value)*

2. ***Regression and Statistical Modeling (3 weeks)***

- *Data preprocessing: centering, scaling, normalization*
- *Simple and multiple linear regression*
- *Curve fitting and model evaluation (R^2, RMSE, residual analysis)*
- *Variable selection: stepwise methods, variance inflation factor (VIF), information criteria (AIC)*
- *Cross-validation*

3. ***Design of Experiments (DoE) (2 weeks)***

- *Definitions and historical background*
- *Classification of experimental designs*
- *Fundamental concepts: factor, response, interaction, repeatability*
- *Introduction to full and fractional factorial designs (2^k designs)*

4. ***Two-Level Full Factorial Designs (2^k) (2 weeks)***

- *Design construction: experimental matrix*
- *Data processing: effect calculation matrix*
- *Statistical analysis: linear regression, error estimation, effect testing, analysis of variance (ANOVA), and empirical model construction*
- *Optimization and validation*
- *Practical applications using software tools (JMP, Statgraphics, Modde, etc.):*

- *polymerization processes (synthesis and characterization), macromolecular chemistry (compounding prior to polymer processing), inorganic formulations, etc.*

5. Central Composite Designs (CCD) (2 weeks)

- *Design construction: experimental matrix*
- *Data processing: effect calculation matrix*
- *Statistical analysis: regression, error analysis, effect testing, ANOVA*
- *Empirical modeling, optimization, and validation*
- *Practical applications using software tools (JMP, Statgraphics, Modde, etc.)*

Other Experimental Designs (3 weeks)

- *Fractional factorial designs / screening designs*
- *Mixture designs*
- *Practical applications: analysis of real data in materials chemistry (formulation, etc.): selection of an experimental design, data collection or simulation, modeling, and interpretation*
- *Writing a concise report summarizing the results of experimental designs*

References *(Books, Lecture Notes, Websites, etc.)*

Jacques Goupy: Design of Experiments: Optimization of Experimental Choice and Interpretation of Results, Dunod, 5th edition, 2017

Sado, G., & Sado, M. C.: Design of Experiments – From Experimentation to Quality Assurance, Afnor, 2000

Tinsson, W.: Design of Experiments: Statistical Construction and Analysis, Springer Science & Business Media, 2010

Goupy, J., & Creighton, L.: Introduction to Design of Experiments, Hachette, 3rd edition, 2006

Droesbeke, J. J., Fine, J., & Saporta, G. (Eds.): Design of Experiments: Applications to Industry, Editions Technip, 1997

Linder, R.: Design of Experiments: An Essential Tool for Experimenters, Presses des Ponts, 2005

Semester: 2

Teaching Unit (TU): Methodology

Course: Artificial Intelligence and Machine Learning 2

Course Objectives

The objective of this course is to deepen students' knowledge of machine learning by introducing advanced concepts such as deep learning, neural networks, generative models, and interpretability techniques. Through this course, students will be able to apply these tools to the discovery and design of new materials in the field of materials science.

Recommended Prerequisites

Students are recommended to have a solid background in basic machine learning, proficiency in the Python programming language, and a basic understanding of atomic and crystalline structures.

Course Content

1. **Graph-Based Models in Materials Science (3 weeks)**

- Materials as graphs: atoms as nodes, bonds as edges
- Crystal Graph Convolutional Neural Networks (CGCNN)
- Case study: prediction of formation energies

2. **Generative Models for Materials Design (3 weeks)**

- Introduction to Generative Adversarial Networks (GANs) and Variational Autoencoders (VAEs)
- Applications: design of new materials and molecules

3. **Model Evaluation and Interpretability (2 weeks)**

- Evaluation techniques for deep learning models
- Cross-validation and overfitting detection
- Model interpretability: SHAP, LIME

4. **Advanced Machine Learning Techniques (3 weeks)**

- Ensemble models: Random Forests, XGBoost, LightGBM
- Advanced regression and classification algorithms
- Dimensionality reduction: Principal Component Analysis (PCA), t-SNE, UMAP

5. **Advanced Applications in Materials Science (3 weeks)**

- AI-assisted inverse design for materials discovery
- Prediction of advanced properties: elastic moduli, superconducting critical temperature
- Multiscale modeling: coupling AI with molecular dynamics and density functional theory (DFT)

6. **Specialization Mini-Project (Capstone Project) (3 weeks)**

- Students will carry out a project in which they apply AI/ML techniques to solve a materials science problem using the skills acquired throughout the semester

Tools and Libraries Used

- Programming language: Python
- Environments: Jupyter Notebooks
- Libraries: TensorFlow, PyTorch
- Specialized tools: Matminer, Pymatgen

References (Books, Lecture Notes, Websites, etc.)

Ian Goodfellow, Yoshua Bengio, Aaron Courville: Deep Learning – MIT Press, 2016
François Chollet: Deep Learning with Python – Manning Publications, 2017
D. K. Jha, T. Chen, M. Tan, H. Chen: Machine Learning in Materials Science – Springer, 2018
Kristin Persson et al.: Data Science for Materials Discovery – CRC Press
Rajiv S. Mishra: Materials Informatics: Methods, Tools, and Applications – Elsevier

Semester: 2

Teaching Unit (TU): Discovery

Course: Semiconductors and Technological Applications

Course Objectives

The objective of this course is to enable students to:

- Understand what a semiconductor is, its physical properties, and the phenomena governing them
- Describe and interpret electronic and optoelectronic processes in semiconductor materials
- Identify the different application fields of semiconductors
- Select the appropriate device for a given application
- Acquire the fundamental background required to pursue academic research or R&D careers

Recommended Prerequisites

Students are recommended to have a solid background in theoretical chemistry, materials physics, semiconductor properties, and their electronic behavior.

Course Content

1. Introduction (2 weeks)

- Physical characteristics of semiconductors
- Types of materials and their application domains

2. Electronic Properties of Semiconductors (4 weeks)

- Band structure
- Band occupancy statistics
- Transport properties
- Recombination processes

3. Junctions and Interfaces (4 weeks)

- Metal/semiconductor junctions
- p–n junctions at equilibrium
- p–n junctions under non-equilibrium conditions

4. Electronic Devices (4 weeks)

- Bipolar transistors
- Field-effect transistors
- Quantum devices
- Emerging materials

5. Optoelectronic Devices (4 weeks)

- Detectors
- Light-emitting diodes (LEDs)
- Laser diodes
- Surface-emitting lasers
- Quantum cascade lasers

References (Books, Lecture Notes, Websites, etc.)

- Charles Kittel: Introduction to Solid State Physics – Dunod, 1998
- N. W. Ashcroft, N. D. Mermin: Solid State Physics – Saunders, 1976
- G. Bastard: Wave Mechanics Applied to Semiconductor Heterostructures – Éditions de Physique, 1992
- J. Pankove: Optical Processes in Semiconductors – Dover, 1975
- F. Lévy: Physics and Technology of Semiconductors – PPUR, 1995
- M. J. Kelly: Low Dimensional Semiconductors: Materials, Physics, Technology, Devices – Clarendon Press, Oxford, 1995
- H. Mathieu: Physics of Semiconductors and Electronic Devices – Dunod, 2001
- S. M. Sze: Physics of Semiconductor Devices – John Wiley & Sons, 1981
- E. Rosencher, B. Vinter: Optoelectronics – Masson, Paris, 1997
- C. Weisbuch, B. Vinter: Quantum Semiconductor Devices – Academic Press, 1991

Semester: S2

Teaching Unit (TU): Discovery

Course: Emerging Polluting Materials

Course Objectives

The objective of this course is to introduce students to the issue of materials considered as emerging pollutants. By the end of the semester, students will be able to:

- Identify materials currently classified as emerging contaminants
- Understand their environmental impact, toxicity, persistence, and bioaccumulation
- Analyze strategies for substitution, recovery, and valorization
- Develop awareness of regulatory frameworks (REACH, RoHS, CLP, etc.)
- Explore sustainable alternatives such as bio-based or recyclable materials

Recommended Prerequisites

Students are recommended to have a solid background in theoretical chemistry, materials properties, as well as fundamental concepts in physics and chemistry of semiconductors.

Course Content

1. **Introduction to Emerging Pollutants (3 weeks)**
- Definitions: emerging contaminants vs. conventional contaminants
- Sources: industrial, urban, agricultural, and medical
- Examples: phthalates, PFAS (per- and polyfluoroalkyl substances), brominated flame retardants, heavy metals, plasticizers, nanomaterials

2. **Environmental Impact of Materials (4 weeks)**
- Material life cycle – Life Cycle Assessment (LCA)
- Persistence, degradability, and bioaccumulation
- Transfer pathways in ecosystems: soil, water, air
- Effects on human health and wildlife

3. **Case Studies of Problematic Materials (4 weeks)**
- Plastics and microplastics
- Volatile organic compounds (VOCs) in paints and adhesives
- Heavy metals in batteries and semiconductor devices
- Nanomaterials: examples (zinc oxide, titanium dioxide, carbon nanoparticles)

4. **Solutions and Alternatives (4 weeks)**
- Safer material design – Design for Environment (DfE)
- Use of bio-based and biodegradable materials
- Advanced recycling and circular economy
- Innovation in non-toxic composites and coatings

References (Books, Lecture Notes, Websites, etc.)

- Jean-Louis Teyssier: Green Chemistry and Sustainable Development
- Collective work: Toxicology and Environment – Chemical Risks and Regulation
- International Organization: Nanomaterials and Environmental Safety, WHO Report
- François Gault: Eco-design of Products and Services: A Prospective and Analytical Approach

Semester: S2

Teaching Unit (TU): Transversal

Course: Materials Selection

Course Objectives

The objective of this course is to enable students to make a well-argued selection of materials for a given application, taking into account physico-chemical properties as well as technical, economic, and environmental constraints.

Recommended Prerequisites

Students are recommended to have basic knowledge in materials science, along with a general understanding of the mechanical, thermal, and electrical properties of materials.

Course Content

1. **General Introduction (1 week)**

2. **Materials and Properties (4 weeks)**

- Materials property charts and maps
- Fundamentals of materials selection
- Case studies in materials selection

3. **Multi-constraint and Multi-objective Materials Selection (4 weeks)**

References (Books, Lecture Notes, Websites, etc.)

Ashby, S.: Materials Selection – Oxford Press, London, 1985

Ashby, M. F.: Materials Selection in Mechanical Design – Elsevier, 2005