# Master Material sciences Specialty "Innovative Materials and Energy Systems"

Graduate Programme E-Mat



Syllabus of the second year for Master's degree



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# **General Overview**

#### INTRODUCTION

E-Mat is a graduate program that takes place in Nantes University. It is an integrated program that opens higher opportunities for those who want to develop their research career path in a doctorate.

This program focuses on the emergence of innovative functional material solutions and optimization of performance, reliability and flexibility for the production, conversion, transfer and storage of energy, energy systems, and advanced devices and technologies. It draws on research excellence in physics, chemistry and engineering of (nano)materials, multi-scale modelling, advanced characterization and thermal management.

It is a part of Master of Material Sciences. **All courses in master 2 are taught in English** and students will have a chance to carry out their research project in an international environment in two of our high-level laboratories (Institute of Materials of Nantes Jean Rouxel, <u>IMN</u> & Laboratory of Thermal Engineering and Energy, <u>LTEN</u>) and to train with specialists on top-level instruments.

#### **CAREERS OPPORTUNITY**

Graduating from our program at the Master or PhD level will open great opportunities to be hired in Research and Development department of industrial companies involved in many sectors, such as:

- Materials
- New and Renewable energies
- Energy production, conversion and storage
- Information and Communication Technologies, Microelectronics
- Transportation/Aerospace.

#### You could become:

- Engineer and executive in Research, Development and Innovation
- Engineer and executive in consulting firms
- Materials engineer
- Academic researcher after a PhD.

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#### PROGRAM LEADERS ON MASTER 2 LEVEL

Pr. Jean-Luc DUVAIL <u>jean-luc.duvail@univ-nantes.fr</u>

Pr Philippe POiZOT <u>philippe.poizot@univ-nantes.fr</u>

Pr Xavier PY <u>xavier.py@univ-nantes.fr</u>



#### SKILLS BASED APPROACH

- 1. Formulate a solution to a complex problem in the field of functional materials, associated processes and energy:
  - ✓ by mobilizing theoretical and technical knowledge and the most relevant models,
  - ✓ by adopting a rigorous scientific approach and reasoning,
  - ✓ by positioning oneself in relation to the state of the art.
- 2. <u>Develop experimentation/modeling in Materials Energy:</u>
  - ✓ using validated protocols or those found in the bibliography,
  - ✓ rigorously implement the experimental or modeling protocol,
  - ✓ respecting good laboratory practice,
  - ✓ by developing the experimental/modeling approach to ensure reproducibility and reliability.
- 3. Analyze data collected in a fundamental or applied research study:
  - ✓ by choosing the most appropriate tools and graphic representations
  - ✓ by critically comparing them with current theories and results found in the bibliographical study,
  - ✓ by exchanging information with specialists if necessary.
- 4. Integrate Research and Development in a professional industrial or academic environment:
  - ✓ deliver a scientific message that is structured, clear and synthetic, both in writing (article, report) and
    orally (team meeting, conference), in one's mother tongue and in English, adapted to the audience and
    context,
  - ✓ respecting the principles of ethics, deontology, environmental responsibility and scientific integrity,
  - ✓ by developing their knowledge and skills through ongoing training and constant monitoring,
  - ✓ by taking part in technological innovation and/or knowledge creation.

#### **TEACHING LOCATIONS**

UFR Sciences et Techniques Campus Lombarderie

2, rue de la Houssinière BP 92208 44322 Nantes Cedex 3

#### **HOW TO APPLY FOR JOINING MASTER 2 E-MAT**

#### Requirements:

Master 2 level is intended for students with a Master 1 degree in physics or physics-chemistry, or equivalent (240 ECTS).

Language requirement:

• TOIEC minimum 800

IELTS: 6.0TOEFL ibt: 80

Or equivalent Graduate of a university in an English-speaking country

Students applying within the framework of a partnership agreement:

The admission procedure and timetable are detailed on:

https://english.univ-nantes.fr/education/application-procedures/exchange-students

Students applying without any partnership agreement:

The admission procedure and timetable are detailed on:

https://english.univ-nantes.fr/education/application-procedures/regular-admissions

#### Scholarship

A welcome grant of **1 500**€ is available to foreign students enrolling at Nantes Université.

Students can also benefit from a monthly grant of 900€ (subject to eligibility).

Students can also apply to excellence scholarships G. Eiffel or other scholarships proposed by their ambassy.

#### **COURSE SCHEDULING**

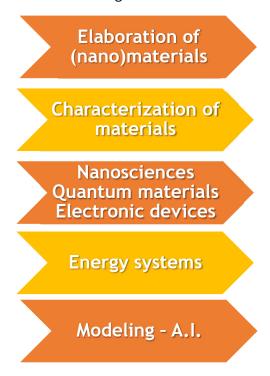
From September to February :	From March to August :
Lectures and practical training	6-month Internship

NB: Students enrolled in a foreign university may do an internship in one of our laboratories at any time of the year, subject to the constraints of their home institution.



#### PROGRAM STRUCTURE

The teaching program is organized in five teaching units detailed in next sections:



# TEACHING UNIT (TU): ELABORATION OF (NANO)MATERIALS 2 (5 ECTS)

#### Advanced chemical synthesis

Affiliated TU: Elaboration of (nano)materials 2		
Duration: 24h Number of ECTS: 2		
Year/semester: M2/S3	3	Language : English
Main teacher	Philippe POIZOT	
Learning objectives	This course trains students in Porous Coordination Polymers, also quoted Metal Organic Frameworks (MOFs), define a class of porous materials that is rapidly growing since 1995. These hybrid solids, which are built up from inorganic building units connected through polytopic organic ligands offer a wide variety of composition and structure, and thus properties.  This course is also focused on the fine control of electrochemical reactions for producing (nano)materials and nanostructured systems.	
Content covered	This course will cover: - the following aspects of MOFs: synthesis, crystal structure, functionalization, porosity and related applications, and structural flexibility The electrodeposition techniques: local pH change, decomposing metal complexes, self-oscillating co-deposition, etc. Practical work: Synthesis and characterization of coordination polymers and MOFs	
Teaching methods	Classroom courses, tutorials, and labwork	
Bibliography		
Prerequisites	Chemistry in solution, acid-base rea	actions, complexing effect, redox reactions

# Nano-microtechnology project

Affiliated TU: Elaboration of (nano)materials 2		
Duration : 20h Number of ECTS: 2		
Year/semester: M2/S3	3	Language : English
Main teacher	Aurélie GIRARD	
Learning Objectives	micro(nano)electronic device by me film deposition in a clean-room.	
Content covered	<ol> <li>Principle of extracting electrical parameters from the DC electrical characteristics of MOS transistors</li> <li>Security rules in the clean room</li> <li>Practical work (part carried out on the CCMO platform in Rennes, 2.5 days):         <ul> <li>Fabrication of an integrated device based MOS technology</li> <li>DC Electrical characterization of the MOS transistors fabricated in CCMO and extraction of the main SPICE electrical parameters (threshold voltage, channel modulation parameter, mobility,)</li> </ul> </li> </ol>	
Teaching methods	Practical work	
Bibliography		
Prerequisitess	Courses on - Advanced physical pro-	cesses and on - Micro-Nanoelectronics

# Advanced physical processes

Affiliated TU : Elaboration of (nano)materials 2			
Duration: 12h	Number of ECTS: 1		
Year/semester: M2/S3	Language : English		
Main teacher	Rim ETTOURI		
Learning Objectives	This module covers the principles of the generic stages in the manufacture of microelectronic devices (6 hours).  A practical section covers TCAD (Technology Computer Assisted Design) initiation using SILVACO, a professionnal software (6 hours).		
Content convered	1. Micro-Nano-Technology processes  - Norms to respect in clean rooms  - Lithography  - Dry and wet etching  - Ion implantation for doping modification  - Oxidation  - Thin film deposition techniques  2. Initiation to Technology Computer Assisted Design using SILVACO		
Teaching methods			
Bibliography			
Prerequisitess	Courses on - Advanced physical processes and on Micro-Nanoelectronics		



# TEACHING UNIT: CHARACTERIZATION OF MATERIALS 2 (3 ECTS)

# Advanced microscopy and spectroscopy

Affiliated TU : Elabor	ration of (nano)materials 2		
Duration: 24h	Number of ECTS: 2		
Year/Semester: M2/	S3	Language : English	
Main teacher	Philippe MOREAU		
Learning objectives	Acquire a good knowledge of SPM, TEM, EELS and XPS techniques Be able to determine which technique to use for what purpose in the context of Innovative Materials and Energy Systems		
Content covered	<ol> <li>SPM (Scanning Probe Microscopy) techniques among which AFM, EFM, KPFM with detailed knowledge of their physical principles and specific examples</li> <li>TEM (Transmission Electron Microscopy) with a special focus on electron-mater interaction (elastic-inelastic), microscope architecture, image formation and interpretation, electron diffraction</li> <li>EELS (Electron Energy Loss Spectroscopy): principle of the spectrum formation, detectors and qualitative interpretation, basis of quantification and its limitation, mapping</li> <li>XPS (X-Ray Photoelectron Spectroscopy): quantitative analysis with special focus on background removal, attenuation length, charging effect and application to PV samples. Deep work on publications found in literature.</li> </ol>		
Teaching methods	Face-to-face lectures as well as training on problems. Support of publications. Practicals with special access to high level instruments		
Bibliography			
Prerequisitess	Basis of light-electron-particle intera Basis of atom and solid state electro		

# Advanced X-ray and neutron diffraction

Affiliated TU: Charact	erization of mate	rials 2	
Duration: 12h	Number of ECTS: 1		
Year/semester: M2/S3	3		Teaching language: English
Main teacher	Olivier HERNAN	IDEZ	
Learning objectives	Advanced characterization of solid-state materials: nuclear and magnetic structures by X-ray and neutron diffraction. Use of synchrotron and neutron diffraction/total scattering techniques.		
Content covered	<b>Part 1.</b> : Production of synchrotron light and neutron beam and comparison of their properties; advanced X-ray and neutron diffraction experiments and structural refinements; total scattering techniques and the pair distribution function. <b>Part 2.</b> : Scientific examples, involving mostly transition metal chalcogenides or clusters, illustrating how such structural analyses may lead to a better knowledge of the nuclear or magnetic structure, for a better understanding of the structure-property relationships.		
Teaching methods	Slide show lecture; Tutorials in groups		
Bibliography	Fundamentals of Crystallography (C. Giacovazzo); Powder Diffraction, Theory and Practice (R.E. Dinnebier, S.J.L. Billinge)		
Prerequisites	Bachelor level in Physics and Chemistry		

# TEACHING UNIT: NANOSCIENCES - QUANTUM MATERIALS - ELECTRONIC DEVICES (6 ECTS)

#### Nanophysics – Quantum materials

Affiliated TU : Nanosciences – Quantum materials – Electronic devices		
Duration: 24h Number of ECTS: 2		
Year / Semester: M2/S	3	Language: English
Main teacher	Jean-Luc DUVAIL	
Learning objectives	electrical properties at the mesosco attention is paid to characteristic p the systems studied. <b>Part 2</b> : Exploration of the main qua	sics that occurs at the nanoscale, emphasizing the opic scale and the spin electronics. Particular hysical lengths in comparison with the dimensions of antum materials families, with a focus on properties tion metal oxides and chalcogenides. Exploitation for nristors, artificial synapses.
Content covered	Part 1: Mesoscopic physics (12h - J. I Fundamentals and confinement II- Electrical properties at the meso III- Fundamentals concepts in spin	scopic scale polarized transport
Content covered	Part 2: Quantum materials (12h - L. Cario, E. Janod) I. Introduction to main families of Quantum materials II. Introduction to strongly correlated materials III. Memories: emerging non-volatile memories IV. Computing paradigm: past, present and future	
Teaching methods	Lectures; case studies on articles fr	om the scientific literature
Bibliography	Review articles from the specialized	d litterature
Prerequisitess	Solid state physics ; cristallography	1

#### Micro-nanoelectronics

Affiliated TU : Nanosciences – Quantum materials – Electronic devices			
Duration: 24h	Number of ECTS: 2		
Year/semester: M2/S3			Language : English
Main teacher	Ahmed RHALLABI		
Learning Objectives	Skills in the electrical properties of CMOS technology and its use in digital and analog applications, Skills in the electrical simulation of basic digital and analog components and functions.		
Content convered	Physics of semiconductors and transport phenomena - MOS transistor - Static and Dynamic studies - CMOS technologie: Electrical studies of basic digital and analog functions - Memory technologies - Project on the design of a static memory for reading and writing		
Teaching methods	Course, applications and project on CAD of SRAM.		
Bibliography	J. Millman and A. Grabel, Microelectronics, McGraw-Hill - International Edition, 1988 P. Molinaro, A. Chriette, Electronique Analogique, Traitement des composants et des circuits, ellipses R. Waser, Nanoelectronics and Information Technology, Wiley-VCH, 2003		
Prerequisites	Physic of semiconductors		



#### Nanomaterials

Affiliated TU : Nanosciences – Quantum materials – Electronic devices			
Duration : 24h Number of ECTS : 2			
Year/semester: M2/S3	3 Language : English		
Main Teacher	Jean-Luc DUVAIL		
Learning objectives	This Course aims to introduce the main families of 0D, 1D, and 2D nanomaterials by emphasizing the relationship beetween: - the synthesis (relevant parameters), - the nanoparticle morphology (with control at the nanoscale) and structure, - the specific properties due to the nanoscale and to the increase of the surface (interface) - their potential for applications.		
	Part A. Metallic nanoparticules (J.L. Duvail) I. Synthesis and related morphologies II. Plasmonic properties (localized surface plasmon resonance; surface plasmon polariton); other properties III. Applications of functional metallic nanoparticles.  Part B. Magnetic nanoparticles (J.L. Duvail) I. Magnetic properties of metal and metal oxide nanoparticles II. Applications of functional magnetic nanoparticles.		
Content covered	Part C. Nanocarbons (C. Ewels) I. Fullerenes (C60,) II. Carbon nanotubes (CNT): growth, structure, properties, applications III. Composites and Fibres IV. Graphene: growth, structure, properties, applications V. Nanodiamond and miscelleneous carbons		
	Part D. 2D Materials (C. Ewels) I. Production and integration of 2D materials (growth, exfoliation,) II. X-enes (phosphorene, silicene,) II. Boron nitride (BN) III. Transition metal dichalcogenides (TMD) IV. MX-enes and 2D oxides		
	Part E. Semiconducting and dielectric nanoparticules (S. Perruchas)  I. Fabrication, main physical properties and potential applications of quantum dots, 0D nanoparticles, nanorods and nanowires  II. Synthesis, functionalisation, optical properties  III. Application for energy conversion, displays, bioimagery and biosensing.		
Teaching methods	Lectures; case studies on articles from the scientific literature		
Bibliography	Review articles from the specialized litterature		
Prerequisites	Solid state physics ; crystallography		

# TEACHING UNIT : ENERGY SYSTEMS (6 ECTS)

#### Photovoltaics 2: New devices

Affiliated TU : Energy sy	stems	
Duration: 28h	Number of ECTS: 2.1	
Year/semester: M2/S3		Language : English
Main teacher	Nicolas BARREAU	
Learning objectives	Introducing students to thin-film PV technologies for renewable energies.  At the end of this course, students will be able to: - understand alternative thin-film technologies to silicon - critically identify the most suitable compounds and architectures for manufacturing a photovoltaic cell - choose the technology best suited to the intended application or use	
Content covered	Thin-film alternatives to silicon:  Part I. CIGS and CdTe thin-film technologies:  Synthesis processes for CIGS and CdTe thin-film materials. Relationships between physico-chemical and electronic properties. Module manufacturing: etching, monolithic integration, innovative architectures. Manufacturing costs. Innovative applications: architectural integration, mobile electronics. Socio-economic impact of inorganic thin-film PV technologies.  Part II. Hybrid dye-sensitized and organic photovoltaic cells:  Operating principles  Materials used and their functions  Relationship between material properties and photovoltaic performance  Large-scale production techniques: inkjet printing and roll-to-roll impregnation  Innovative applications: architectural integration, mobile electronics	
Teaching methods	Lectures, tutorials, in-class dem	onstrations
Bibliography		
Prerequisites	Principles and Applications	

# Electrochemical storage level 2: new devices

Affiliated TU : Energy systems		
Duration: 28h		Nombre d'ECTS : 2.1
Year/semester: M2-S3		Language : English
Main teacher	Philippe POIZOT	
Learning objectives		



Content covered	1. Electrochemical energy storage systems:  - Introduction to electrode shaping techniques  - Advanced electrochemical characterization techniques (PITT, GITT, power measurements)  - Future technologies: new electrode materials and devices  - Supercapacitors and hybrid systems  2. Hydrogen vector:  - Production, processing and characterization  - Storage and distribution  3. Practical aspects:  - Assembly and performance evaluation of semi-commercial devices (batteries and supercapacitors)  - Electrochemical impedance spectroscopy and modeling of equivalent circuits (application to fuel cells)	
Teaching methods	Classroom courses, tutorials, and labwork	
Bibliography		
Prerequisites	Fundamentals of electrochemistry, Butler-Volmer equations, Tafel, Diffusion, Cell assembly, Performance assessment of electrochemical generators	

# Thermal energy systems

Affiliated TU : Ener	gy systems		
Duration: 24h		Number of ECTS	: 1.8
Year/semester: M2/S3			Language: English
Main teacher	Xavier PY		
Learning Objectives	At the end of the course, students will be familiar with the main thermal energy systems involved in the energy transition, and with the issues linked to the associated materials in terms of both their properties for use and their environmental impact. They will be able to carry out a materials selection study based on a comprehensive multi-criteria methodology.		
Content convered	The course is dedicated to some of the major thermal energy systems of the energy transition, for which materials-related aspects are crucial. Namely, the systems studied are: thermal energy storages (sensible heat, latent heat, thermochemical), non-concentrated and concentrated solar thermal energy, surface geothermal energy and CO2 capture. The materials involved are studied both for their properties of use and their environmental impact. Particular emphasis is placed not only on material characterization techniques, but also on multi-criteria selection methods. The entire course is also illustrated with current contextual data in terms of material requirements for the energy transition, potential conflicts of use and changes in world markets. Part of the course is dedicated to practical work on the materials and systems under consideration.		
Teaching methods	The training will be based on lectures, practical work on group, critical reading and discussion of documents.		
Bibliography	Students will be invited to follow and read European and international expert reports on the energy transition and related processes (IEA, IPCC, ADEME, etc.). Specific academic publications will also be provided for group reading and discussion.		
Prerequisites	Basic knowledge on energy production, conversion and storage.		

# TEACHING UNIT : MODELING 2 (6 ECTS)

# Multiphysics modeling 2

Affiliated TU: Modeling 2			
Duration: 24h		Number of ECTS: 2	
Year/Semester : M2/S3 Language : French / English			
Main teacher	Stéphane CUENOT		
Learning objectives	<ul> <li>The student will be able to:</li> <li>master the modeling steps of a simple multiphysics problem</li> <li>master the optimization of the mesh to ensure the convergence of the numerical solution by controlling the compromise between precision and computation time</li> <li>know how to structure the numerical resolution steps of a complex multiphysics problem</li> </ul>		
Content covered	2D and 3D modeling of simple and complex multiphysics problems Control of boundary conditions, mesh and solvers for coupled physical problems Weak and strong coupling of the physical modules used Control of the convergence of the numerical solution, optimization of the mesh Multi-physics problems solved in stationary, transient and parametric regimes Post- processing and analysis of numerical results.		
Teaching methods	Students work individually on practical multiphysical modeling work, before developing a micro-modeling project in pairs.		
Bibliography			
Prerequisites	Physical and multi-scale modeling		

#### Quantum mechanical modeling of electronic interactions

Affiliated TU: Modeli	ng 2			
Duration: 24h		Number of ECTS: 2		
Year/semester: M2/S	S3		Language: English	
Main teacher	Camille LATOUCHE			
Learning Objectives	In this course, the theoretical foundations necessary for understanding, implementing, and interpreting ab initio simulations for molecular and solid materials will be presented, particularly focusing on methods based on wave function (WF) and density functional theory (DFT). Upon completion of this course, the student will be able to:  - determine the most appropriate method to study a material and its properties e.g.: simulate absorption spectra in the UV and vibrational spectra)  - understand and rationalize observed properties to guide experimentalists towards the synthesis of materials with optimized properties  - interpret and analyze modeling results from the scientific literature.			
Content convered	Part 1: Quantum modelling of electrons in crystals  1.Reminder: electrons in crystals; reciprocal space  2. Bloch electrons; Born von Karman boundary conditions; Brillouin zone  3. Electronic structure: the tight binding model  4. Electronic correlation: towards magnetism  5. Quantum transport using non equilibrium Green functions  Part 2: Density Functional Theory  1. Introduction to Quantum modelling in Chemistry and Physics: from HF to DFT  2. Computations: from relaxation to properties  3. How to interpret properties through computations  4. Beyond DFT			
Teaching methods			P). A distance project will also be included.	



Bibliography	Introduction to Computational Chemistry, F. Jensen; Modern Quantum Chemistry, A. Szabo and N. Ostlund; Quantum Chemistry, I. N. Levine; Essentials of Computational Chemistry (Theories and Model), C. Cramer
Prerequisites	

# Artificial Intelligence for materials discovery and design

Affiliated TU: Modeling 2			
Duration: 24h	Number of ECTS : 2		
Year/semester : M2/S3		Language : English	
Main teacher	Isabelle BRAEMS-ABBASPOUR		
Learning objectives	material with given properties - Use tools for data mining, machin (genetic algorithms) - Familiarize themselves with the t	ges of AI in materials science and analyze these data when searching for a ne learning and deep learning, and optimization	
Content covered	Materials informatics is a recent discipline that applies some advanced tools from informatics to materials science and engineering in order to improve efficiently the understanding, use, design, selection, and discovery of materials. It includes combinatorial chemistry, materials property databases, and tools from artificial intelligence (machine learning, deep learning) to accelerate both the discovery and design of new materials.  1. Introduction to AI, material databases, data mining 2. Machine learning 101 3. Deep learning in materials science 4. Crystal structure prediction for solids and carbon molecules 5. Introduction to generative AI		
Teaching methods	Individual learning in the form of pra academic research papers	actical work directly linked to the course; study of	
Bibliography			
Prerequisites			

# TEACHING UNIT: PREPARING FOR PROFESSIONAL INTEGRATION (4 ECTS)

Innovation, transitions and project management under high uncertainty

Affiliated TU: Preparing for professional integration			
Duration: 21h Number of ECTS: 3.2			
Year/semester: M2/S4 Language: mixed English and French (possibility of using the Omist translation to			
Main teacher	Mathias GUERINEAU		
Learning Objectives	At the end of the course, students will be able to:  - Understand local, national and international innovation systems  - Adopt a critical and analytical view of technologies  - Understand and integrate technological, human and societal issues linked to transitions  - Responding to a call for projects  - Plan and organize over time  - Manage a team in a situation of uncertainty  - Use specific project management tools to deal with uncertainty		
Content convered	Contemporary project management practices: - organization of research based on calls for projects and the inherent difficulties, - discovery and practice of contemporary project management tools, - discovering agile methods for working under uncertainty, etc.  Innovation management in transitions: - the place of technologies in transitions, - dissemination and acceptability of innovations & technologies in society, - taking ecological constraints into account in innovation models.  3 issues are particularly addressed in this course:  Defining and managing innovation; The question of spatial anchoring in innovation ecosystems and; the question of paradigm shifts (growth, ecology, sobriety, etc.) around innovation.		
Teaching methods	Face to face for notions and theories, case studies, debates		
Bibliography			
Prerequisites			

#### Thematic school

Affiliated TU: Preparing for professional integration			
Duration : h		Number of ECTS: 0.8	
Year/semester: M2/S3 Language: English		English	
Main teacher	Jean-Luc Duvail, Philippe Poizot, Xavier Py		
Learning Objectives	At the end of the course, students will be able to:  - Manage the organization of the day(s) related to the event.  - Develop interpersonal skills through interactions with event guests.  - Strengthen the ability to work independently.		
Content convered	Variable topics		
Teaching methods	Face to face for notions and theories, case studies, debates		
Bibliography			
Prerequisites			



#### TEACHING UNIT: INTERNSHIP (30 ECTS)

The internship plays an important role in the E-Mat Master's curriculum, and is based on close interaction between research and technological innovation. Students will spend between 4 and 6 months working in a national or international research team or industry.

Mobility of students enrolled in the E-Mat Master's program during the internship:

This GP encourages international mobility for students by making available to them the international network of teacher-researchers from the two partner laboratories.

Students are eligible for a mobility grant of between €500 and €700 per month, depending on the target country. They are also eligible for a €1,000 relocation grant.

Hosting foreign students for internships in our partner laboratories:

Foreign students wishing to do an internship in one of our partner laboratories should send their application, together with their CV and a summary of their areas of interest, to the program coordinators. If the application is deemed admissible, they will be offered an interview to explain their objectives.

# Nantes Université