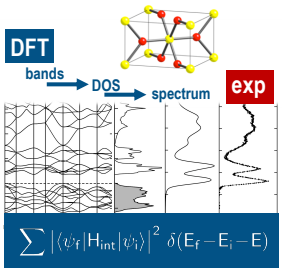
SCIENCES SORBONNE UNIVERSITÉ

MASTER
Physique fondamentale et applications

SMNO nanomat master

M2 – SMNO-nanomat – MIM

Title:	Materials Investigation Methods: experiments and modelling (MIM)	
	Apogée code: MU5PYM05 **Number of credits:** 6 **Teaching hours:** 40h (exp. part) + 20h (th. part) courses	

Lecturers: "Exp." part	Delphine CABARET (coordinator) IMPMC– 23-24 – 427 delphine.cabaret@sorbonne-universite.fr	Gwenaëlle ROUSSE Collège de France	Paola GIURA IMPMC – 23-13 – 413	Marie D'ANGELO INSP -22-32 – 213
	Nicolas MENGUY IMPMC – 23-24 – 412	Dimitri RODITCHEV LPEM-ESPCI	Guillaume RADTKE IMPMC– 23-24 – 421	
Lecturers: "Modelling" part	Marco SAITTA (coordinator) IMPMC – 23-22 marco.saitta@sorbonne-universite.fr	Fabio PIETRUCCI IMPMC – 23-24 – 304		

Objective	This course introduces experimental and theoretical methods for materials properties investigation from the physicist point of view. The goals are the following: ○ to provide the graduate student, whether more experimentalist or more theoretician, a good knowledge and comprehension of the physics behind the experimental and theoretical approaches currently used in materials science ○ to make the graduate student capable to define and carry out experimental/theoretical protocols to address a scientific problem in materials science ○ to provide a strong physical background for the practical works that are carried out in the LabS teaching unit
Content	• Description of the probes experimentally used to investigate materials properties (photons from infra-red to hard X-rays, electrons and thermal neutrons); presentation of the light-matter interactions including the connections between microscopic mechanisms and macroscopic responses; interaction cross sections, electronic transition selection rules, angular dependence • Presentation of various experimental methods, dedicated to studies of structural, electronic and vibrational properties of materials (bulk crystals, nanosized materials, surfaces, …): ○ Common lectures on x-ray and neutrons diffraction, IR absorption spectroscopy, Raman scattering, x-ray and neutron inelastic scattering, photoelectron spectroscopy (XPS, UPS) ○ Option 1: Specialization on structural, electronic and vibrational properties of materials using TEM, EELS and XAS. ○ Option 2: Specialization on electronic properties of surfaces and 2D materials using ARPES, STM and STS. • Description of the theoretical methods used to model/predict materials properties (ab initio *vs* classical): ○ Density Functional Theory (DFT), Density Functional Perturbation Theory (DFPT), ○ Statistical sampling and thermodynamics, Metadynamics ○ Atomistic simulations (Monte Carlo and Molecular Dynamics simulations)
Prerequisites	Geometrical crystallography: lattice points and motif, lattice systems, Bravais lattices, conventional crystal cells, crystallographic point groups, space groups, Miller indices, crystal direction, lattice plane, Bragg planes, reciprocal lattice, Brillouin zone, etc. Maxwell equations, quantum mechanics and atomic physics (time-dependent perturbation theory, Fermi golden rule, harmonic oscillator, second quantization, Dirac and Schrödinger representations, spherical harmonics, kinetic moments coupling), statistical mechanics
Examination	"Exp." Part: final written examination "Modelling" part: final written examination