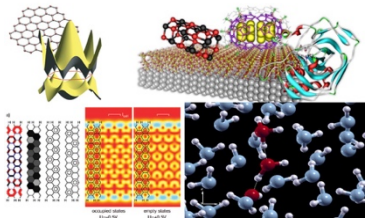
SCIENCES SORBONNE UNIVERSITÉ

MASTER
Physique fondamentale et applications

SMNO nanomat master

M2 – SMNO-nanomat – CMS

Title:	Computational Materials Sciences (CMS)	
	Apogée code: MU5PYM14 **Number of credits:** 6 **Teaching hours:** 20h lectures, 12h tutorials and 20h project	

Lecturers and tutorials/project supervisors:	Marco SAITTA (coordinator) IMPMC – 23-24 – 309 marco.saitta@sorbonne-universite.fr	Fabio PIETRUCCI IMPMC – 23-24 – 304	Guillaume FERLAT IMPMC – 23-24 – 423
	Fabio Finocchi INSP – 22-12 – 506	Simon HUPPERT INSP – 22-12 – 504	Jean-Noël AQUA INSP – 22-12 – 415

Objective	This course presents a deep overview of advanced computational methods to study the physical and chemical properties of materials, predict their properties, and design novel ones with better technologically-oriented properties. The goals are the following: • to acquire a good knowledge and comprehension of the physical and chemical basis of the state-of-the-art simulation methods used in materials science, • to achieve a 20h-computational project using advanced simulations codes, currently used in computational materials science, • to be able to present the results within an "article-like" written report and a "conference-like" oral presentation.

Content	The master unit encloses lectures (20h), introducing numerical tutorials (4h each) and a numerical project (20h).
	• The **lectures** describe the theoretical methods (ab initio, statistical, classical) used to model/predict materials properties:
	  ○ Density Functional Theory (DFT), Density Functional Perturbation Theory (DFPT),
	  ○ Statistical sampling and thermodynamics, Metadynamics
	  ○ Atomistic simulations (Monte Carlo and Molecular Dynamics simulations)
	• The preliminary **tutorials** aim at applying fundamental concepts of solid-state physics and mechanical statistics using specific computational codes.
	• The goal of the computational **project** is to encourage students beyond the strict "school" framework, to conduct a real research effort partly autonomous, on problems that have been chosen among actual research topics (see in section "contents" the list of project keywords) and using concepts that they have learned during more specialized courses or will learn on the job.
	The tutorials and computational projects will be carried out by teams-of-two, thus introducing students to collaborative research, sharing their respective know-how and encouraging informal discussions.
	Project keywords: ferroelectric transitions, graphene, nano-crystal shape, Jahn-Teller distortion, magnetic alloys, thermal expansion, metadynamics, crystals under high pressures, growth of quantum dots, fractal/compact growth, glassy systems, vibrations in minerals, active matter

Prerequisites	Geometrical crystallography: lattice points and motif, lattice systems, Bravais lattices, conventional crystal cells, crystallographic point groups and space groups, crystal direction, lattice plane, reciprocal space, Brillouin zone, etc. Quantum mechanics, statistical physics and atomic physics.
Examination	Written examination Project evaluation: report and oral presentation
Nota Bene	The CMS teaching unit is designed for students enrolled in the Master of Chemistry. Students enrolled in the Master of Physics follow this course within both MIM and LabS SMNO master units.