

PHD PROGRAMME IN PHYSICS, ASTROPHYSICS, AND APPLIED PHYSICS
UNIVERSITÀ DEGLI STUDI DI MILANO
PhD Cycle 41 (2025-2026)

All lectures will be given in English.

Course title	HPC@Unimi: INDACO for molecules and solids
Teacher in charge of the course	Fratesi Guido
List of the teachers of the course	Fratesi Guido, Unimi-Dept. of Physics; guido.fratesi@unimi.it Martinazzo Rocco Unimi-Dept. of Chemistry; rocco.martinazzo@unimi.it Alessi Alessio, TAB Unimi; alessio.alessi@unimi.it Bensi Michele, TAB Unimi; michele.bensi@unimi.it
Training objectives	Fundamentals of computers and networks, UNIX; installation and configuration of programs to access Indaco; software optimization and management. The electronic problem, introduction and definition. Chemical bond and electronic properties; molecular structure and transformations. Methods for solid state physics; application to periodic and non-periodic systems.
Prerequisites	Quantum mechanics. Basics of structure of matter, molecular physics and physics of solids. Basics of statistical mechanics (Boltzmann, Fermi-Dirac, Bose-Einstein distributions). The course is also suitable for students without prior knowledge of electronic structure simulations.
Detailed course program	This course provides an introduction to HPC with special emphasis given at the facilities available within UNIMI (INDACO), and to its application to the calculation of electronic, structural, and spectroscopic properties of molecules and solids. HPC at Indaco. Fundamentals of computers and networks, UNIX; installation and configuration of programs to access Indaco; software optimization and management. The electronic problem. Introduction: Born-Oppenheimer approximation, potential energy surfaces and their topology, adiabatic vs. non-adiabatic dynamics. Electrostatic Hamiltonian, antisymmetry principle, Slater determinants, spin-symmetry. Methods based on the electronic wavefunctions: Hartree-Fock and post-HF methods. Density functional theory, Kohn-Sham method, Exchange-correlation functionals. Time-Dependent Density Functional Theory. Methods for molecules. Atom-centered basis sets. The chemical bond: the hydrogen molecule, valence bond vs molecular orbital theories, localization, natural bond orbitals. Introduction to Gaussian/GAMESS. Electronic structure and molecular properties (with exercises). Geometry optimization,

	transition-state search, intrinsic reaction paths, normal mode analysis (with exercises). Methods for the solid state. The atomic pseudopotential and the projector augmented wave. DFT in a plane wave basis set. Computational issues. Self-consistency and convergence. Brillouin zone integration. Lattice vibrations: frozen phonon and density functional perturbation theory. Introduction to the Quantum-ESPRESSO simulation package. Application to bulk systems. Electronic properties of elemental crystals. Phonons. Application to non-periodic systems: surfaces, molecules. Exercises.
Examination modalities	Homework solution of individually assigned numerical problems. Oral discussion based on these problems and on other topics seen during the lectures.
Preliminary schedule	Between June and July 2026 Course enrolment deadline: December 27, 2025.