PHD PROGRAMME IN PHYSICS, ASTROPHYSICS, AND APPLIED PHYSICS UNIVERSITÀ DEGLI STUDI DI MILANO

PhD Cicle 41 (2025-2026)

All lectures will be given in English.

All lectures will be given in Englist Course title	Quantum Theory of Matter
Teacher in charge of the course	Manini Nicola
List of the teachers of the course	Manini Nicola, University of Milan, nicola.manini@unimi.it Onida Giovanni, University of Milan, giovanni.onida@unimi.it Parola Alberto, University of Insubria, alberto.parola@uninsubria.it Achilli Simona, University of Milan, simona.achilli@unimi.it
Training objectives	Familiarizing the student with the main theoretical concepts and state-of-the-art methods for the calculation of structural and spectroscopic properties of molecules and solids.
Prerequisites	Practical quantum mechanics (Schrodinger equation, and its solutions in standard problems such as a free particle, the quantum harmonic oscillator, the one electron atom; canonical interpretation of the wave function; perturbation theory); basic concepts of electromagnetism and structure of solids.
Detailed course program	General methods and concepts. Symmetries in physics and group theory. Subgroups. Group representations. Examples. Product groups. Representation reducibility. Fundamental theorems of the group representation theory. Representation characters. Examples and applications to problems in condensed matter and solid-state physics. Born Oppenheimer separation. Adiabatic-diabatic transformation. Examples and applications. Ehrenfest dynamics. The many-electrons problem Many-body Hamiltonian for N electrons and M nuclei. Summary on the variational principle and its application within the Hartree-Fock method. Matrix elements of 1 body and 2 body operators on determinantal states. Electron density and density matrix, and their functional derivatives. Total energy and double counting. Excitation energies and Koopman's theorem. Density Functional Theory: Hohenberg-Kohn, Thomas-Fermi, Kohn-Sham. Similarities and differences wrt HF. Local and semi-local density functionals. Theoretical tools: self-consistent ab-initio methods. Choice of the basis set. The pseudopotential description of core states. Periodic boundary conditions. Time-dependent DFT Spectral functions. Self-energy. Equation for the poles of the one-electron Green's function. Hedin's equations. The GWGamma scheme. The GW approximation. One-shot GOWO. GW implementation in open-source codes. Hybrid functionals. Excitonic effects in optical absorption spectra. Bethe-Salpeter equation. Local fields.

	 Strongly correlated electron systems Role of the electron-electron interaction in the electronic structure of solids. Introduction to the second-quantization method. Fock space, creation and annihilation operators, second-quantized Hamiltonian for the electron gas. Electronic structure of transition metals. Hubbard model. Mott transition. Strong and small coupling limits of the Hubbard model. Origin of antiferromagnetism in condensed matter. The Heisenberg model. Metal-insulator transition in the Hubbard model: mean-field theory. Hubbard model with attractive interactions: superconductivity. Analogies with the BCS theory.
	Final hands-on Computational-lab with examples of application of an open-source DFT ab initio code for the calculation of electronic properties of molecular and crystal systems.
Examination modalities	The student can opt between (i) a traditional interview covering all course contents, (ii) a seminar presenting a focused topic studied through a few journal papers, or (iii) the discussion of an original calculation.
Preliminary schedule	March 2026-May 2026 Course enrolment deadline: December 27, 2025.