Finanziato dall'Unione europea NextGenerationEU
Ministero dell'Università e della Ricerca
Italiadomani PIANO NAZIONALE DI RIPRESA E RESILIENZA
Scuola di Studi Superiori "Carlo Urbani"

INTRODUCTION TO THE DENSITY FUNCTIONAL THEORY: PRINCIPLES AND PRACTICE

Advanced training Course

Dr. Fabio Finocchi

Format: Blended (Camerino + online)

Where: Teaching Laboratory, Physics Building

When: April–May 2026

Registration deadline: 08 April 2026

Places: Max. 30 students

Enrolment Form

Organized by UNICAM
within the framework of the EFC Project

Detailed program

Theoretical Lectures

1. **Thu 9/4** 14:00-16:00
   Introduction. Functionals vs. functions. The Raleigh-Ritz variational principle. Hohemberg-Kohn theorems for the ground state. Electron density and density matrix.

2. **Fri 10/4 am** 11:00-13:00
   The construction of a functional: the Thomas-Fermi-Hartree functional. Exchange-correlation energy in the Local Density approximation. Ground state via functional minimization. The effective one-particle potential.

3. **Mon 13/4 pm** 14:00-16:00
   The Kohn-Sham equations. The meaning of eigenvalues of the Kohn-Sham equations. Varying the number of electrons. Chemical potential and their derivatives. Fractional occupations. HOMO-LUMO gap in DFT.

4. **Thu 16/4 pm** 14:00-16:00
   Generalization of DFT to systems with net spin polarization. Exchange energy of the uniform electron gas in the Hartree-Fock approximation. The exchange-correlation hole.

5. **Fri 17/4 am** 11:00-13:00
   The jungle of exchange-correlation functionals. Classes of functionals and most used ones.

6. **Thu 23/4 pm** 14:00-16:00
   The Hellmann-Feynman theorem in the DFT. Generalized forces. Atomic forces and pressure. Optimization methods: structure.

7. **Mon 27/4 am** 9:00-11:00
   Born-Oppenheimer first-principles (DFT-based) molecular dynamics. Constant-temperature molecular dynamics through the Langevin equation with atomic forces from DFT.

8. **Thu 30/4 pm** 14:00-16:00 and 16:00-18:00
   Introduction to the Density Functional Perturbation Theory (DFPT). Perturbation expansion to all orders. Second-order perturbations. The Sternheimer equation within DFPT.

9. **Mon 4/5 am** 9:00-11:00
   Response functions via DFPT: Elastic constants and mechanical properties of crystals. Phonons, dielectric constant, effective charges. Connection with experiments: computing infra-red spectra.

EXAM 1: short written test

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Detailed program

Computational Lab Sessions

1. **Mon 13/4 am** 9:00-11:00
   Ground state of the He atom via the Raleigh-Ritz variational principle. Correlation energy.

2. **Mon 20/4 am** 9:00-11:00
   How to solve the Kohn-Sham equation in practice. Finding the fixed point of the self-consistent field. Basis sets: localized and extended functions. Plane waves. Core and valence electrons in atoms. Ionic pseudo-potentials. (All of those topics will be explained by a hands-on dealing with the Al crystal)

3. **Mon 20/4 pm** 14:00-16:00
   Presentation of the simulation projects and choice by the students
   Project/1 : Start

4. **Fri 24/4 am Project/2** 11:00-13:00

5. **Mon 27/4 pm Project/3** 14:00-16:00

6. **Thu 30/4 pm Project/4** 14:00-18:00

7. **Mon 4/5 pm Project/5** 14:00-16:00

8. **Thu 7/5 pm Project/6** 14:00-16:00

9. **Fri 8/5 am Project/7** 11:00-13:00

10. **Mon 11/5 am Project/8** 9:00-11:00

11. **Mon 11/5 pm Project/9** 14:00-16:00

12. **Thu 14/5 pm Project/10** 14:00-16:00
    (optional : free time for questions and discussion or for running further simulations)

EXAM 2: written report

Each “slot” consists of 2 hours. The computer sessions may be continued at the students' convenience beyond the scheduled time. Instructions on how to install and run the “Quantum Espresso” package on the students’ computers will be provided before starting the computer sessions.

Participants must have a personal laptop and an internet connection

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