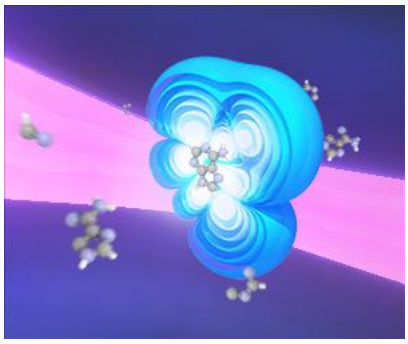
PhD Lecture series:



Introduction to DFT and TDDFT

Tuesday, 3/10/2023, 14:30 - 17:30
Thursday, 6/10/2023, 14:30 - 17:30
Tuesday, 10/10/2023, 14:30 - 17:30
Thursday, 12/10/2023, 14:30 - 17:30
Tuesday, 17/10/2023, 14:30 - 17:30
Thursday, 19/10/2023, 14:00 - 19:00 (hands-on)

Aula D, DIFC, Via Archirafi 36

Prof. Umberto De Giovannini

This short course serves as an introduction to the fundamental principles of Density Functional Theory (DFT) and Time-Dependent Density Functional Theory (TDDFT). Originating from quantum mechanics, DFT offers a more computationally feasible approach to studying the microscopic properties of atoms, molecules, and solids. By reformulating the many-body Schrödinger's equation in terms of electron density rather than the wavefunction, DFT drastically reduces computational costs, making it a widely adopted tool in physics, chemistry, materials science, and biochemistry.

While DFT excels in determining structural properties, it faces limitations in addressing time-dependent processes and excited-state properties of electronic systems. To bridge this gap, Time-Dependent Density Functional Theory (TDDFT) has been developed. The course covers the foundational concepts and theorems of both DFT and TDDFT, offering students a theoretical understanding of these methods.

Moreover, the course provides practical, hands-on experiences by introducing students to the utilization of the Octopus DFT/TDDFT code. Participants will gain practical insights into implementing these theories, enhancing their skills in electronic structure theory.