



FIM-S3 SEMINAR

From weak to strong electric fields: the linear and nonlinear optical response of atoms, molecules and solids

Thursday July 4th, 2024 – 15.00 (sharp) S3 Seminar Room, 3rd Floor, Physics building

Remote link: Teams

Speaker Eleonora LUPPI – Sorbonne University and CNRS, Paris, France

Abstract

The theoretical advancements in linear and nonlinear optics, from weak to strong electric fields, are fundamental for deepening our comprehension of the optical response of atoms, molecules, and solids. In the linear response regime (weak field), I will discuss new theoretical developments for describing photoionization and core resonances using B-splines and Gaussian basis sets in the framework of range-separated Time-Dependent Density Functional Theory (TDDFT). In the second- and third-order regimes (weak field), I will discuss Second-Harmonic Generation and Electric Field-Induced Second Harmonic processes for bulk systems within the framework of TDDFT. Finally, beyond perturbation theory (strong field), I will discuss High-Harmonic Generation for molecules using Quantum Chemistry approaches extended into the time domain.

Host: Alice Ruini and Elisa Molinari









THE EXASCALE



