Giovedi 8 novembre in aula Rasetti ore 14.45: Seminario del vincitore della procedura concorsuale RTDA Dr. José A. Flores Livas

Titolo: In silico Design of Quantum Materials

Abstract:

In order to progress towards building a scalable and robust quantum computer, we require materials with a distinct set of features,
such as specific photon-mediated interactions and desired superconducting properties.
It is imperative to accelerate our understanding of these features to discover novel platform materials for quantum computing and to consolidate
the emergent field of Quantum Information. During my talk I will address, what are Quantum Materials (QM) and how do we study them.
The main objective of the project I present is to design, discover and engineer in silico materials for quantum computing applications.
To achieve the main objective, first we will implement new computational approaches to identify candidate materials that may host novel qubits.
Potential qubits can be formed by point defects in solids that result in emergent deep electronic states. We aim to develop a workflow that allows
us to accelerate the discovery of such defects and to verify their suitability to act as a qubit. Zero-phonon photoluminescence spectra and hyperfine
tensors calculations will be incorporated into our algorithms. The objective is to guide experimental efforts towards novel quantum-light sources,
bringing a palette of possibilities to the field of solid state systems based quantum computers.
Second, we will derive and implement an extension of SuperConducting Density-Functional Theory (SCDFT), that includes spin-orbit (SO) coupling
and a spin-triplet pairing mechanism. Both quantities are essential to study topological superconductors. When SO-interactions in materials are strong enough,
the order of electronic energy bands is modified, and a subtle interplay between superconductivity and topologically ordered phase arises.
Having a computational tool to study these interactions ab initio is fundamental to engineer topological phases
and to identify exotic quasiparticles such as Majorana fermions in solids, considered as a promising path towards topological quantum computing.