UNIVERSITÀ DEGLI STUDI DI TORINO

Dipartimento di Fisica

Seminar

Prof. Marco Govoni

Università di Modena e Reggio Emilia

First principles studies of quantum point defects

Friday, April 14th h 14:30

Aula Wataghin – Dipartimento di Fisica

The robust description of excited states for complex heterogeneous systems is the cornerstone of a computational framework that enables the modelling of materials for sustainable energy and quantum information science applications. I will present the simulation of optically activated processes, e.g., optical absorption and photoemission, in materials using a hierarchical modeling approach that relies on the combination of density functional theory, many-body perturbation theory, and multi-reference methods. I will focus on simulations of point defects in diamond and silicon carbide, which are of interest for the realization of quantum technologies. These examples benefit from the use of the latest developments in high-performance computing architectures, which include pre-exascale capable machines and quantum processors.

The speaker

Marco Govoni is an assistant professor in the department of physics, computer science, and mathematics of the University of Modena and Reggio Emilia. He is also a visit assistant professor in the Pritzker school of molecular engineering at the University of Chicago and a visiting scientist in the materials science division at Argonne National Laboratory. He is recipient of the 2020 DOE Early Career Award. He graduated in physics and obtained his PhD in nanoscience and nanotechnology at the University of Modena and Reggio Emilia. He was a postdoctoral researcher at the Italian leadership computing facility CINECA, at the University of California Davis, at the University of Chicago and Argonne National Laboratory. His expertise is in theoretical and computational condensed matter physics.