NANO COLLOQUIA 2022 - S3 SEMINAR

First principles characterization of defect states in emerging materials for next-generation technology

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ONLINE - https://meet.goto.com/173227901

Speaker
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Abstract
Information and communication technologies have been historically powered by silicon. The current major worldwide drive for big data, machine learning and quantum computing threatens to overwhelm Si-based resources and architectures. The search for alternative materials and technologies is therefore crucial and it represents a unique opportunity to explore and link materials' properties and performances in unexplored architectures.
In this upcoming process, many of the emerging candidates for next-generation technology include disrupting solutions for in-memory computing and synaptic electronics, based on chalcogenides, metal-oxides and other non-Si-based materials in their crystalline, amorphous or disordered phases. Characteristic high densities of defect states play a pivotal role in transport in these systems – even more than in traditional electronics – such that defects and traps govern long-term stability and performances of devices. Therefore, describing, identifying, and controlling defect states is crucial to characterize properties of emerging materials and their interplay with non-standard device architectures, as well as to engineer already known materials to improve their application range.
In this colloquium I will present some of the work we have been carrying on in such direction within the European projects INTERSECT and OpenModel. In particular, I will focus on the study of stability, thermodynamics, diffusion and electronic properties of point defects in crystalline GeSe chalcogenide, a promising system for in-memory computing, and TiO2, well-known material with a wide range of applications spanning form photocatalysis to electrochromics. The investigations have been performed by means of the Quantum ESPRESSO suite of codes and of state-of-the-art high-throughput workflows for first principles condensed matter simulations, part of the AiiDA automated infrastructure.

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