



Università
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e Nanosistemi

The shape of things to come: first-principles simulations driving discovery and innovation

23 aprile 2024, ore 11.00

Aula conferenze Orio Zanetto, Edificio Alfa ed in videoconferenza al link: <https://unive.zoom.us/j/86367419924> - password: seminar1

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Computational science has benefited for many decades from the algorithms and the hardware that have made it one of the greatest accelerators of research, with results and impact that run deep in scientific discovery and technological innovation. This is particularly true for first-principles simulations, which address directly the quantum mechanics of interacting electrons and nuclei and have become one of the most widely used and widely misused tools in research. I'll first illustrate the key challenges and opportunities that this new kind of science faces: 1) of predictive accuracy, with simulations able to capture faithfully the quantum nature of electrons and nuclei; 2) of realistic complexity, aiming to describe ever more realistic systems; and 3) of materials informatics, leveraging the

disruptive capabilities of machine learning and data mining, quantum computing, and artificial intelligence. I'll then highlight some of the key efforts we are targeting: addressing the electronic structure of compounds with strongly localized electrons, developing mesoscopic equations and formulations that bring atomistic and quantum precision to the macroscopic scale, and delivering automated capabilities that can be externalized and then orchestrated by human and not-so-human players. Some case studies will cover the design and discovery of materials for energy (Li-ion cathodes and solid-state conductors) and materials for information-and-communication technologies (2D and 1D materials, topological insulators, and superconductors).