



UNIVERSITA' DEGLI STUDI DI PAVIA

DOTTORATO DI RICERCA IN FISICA

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Aula 102 "L. Giulotto", ore 16.00

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To see a world in a grain of sand

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Abstract: Quantum-mechanical simulations have become dominant and widely used tools for scientific discovery and technological advancement; since they are performed without any experimental input or parameter they can streamline, accelerate, support or replace actual physical experiments. This is a far-reaching paradigm shift, substituting the cost- and time-scales of brick-and-mortar facilities, equipment, and personnel with those, very different, of computing engines, and aiming at the ultimate goal of understanding, predicting, and designing from first-principles the properties and performance of novel or complex materials and devices.

I will offer my perspective on the current state-of-the-art in the field, and its power and limitations, following it with two examples. The first one is dedicated to the discovery of novel materials, with a high-throughput search of all known inorganic compounds, finding more than 1800 materials that could be exfoliated in novel 2D monolayers, with intriguing electronic, optical, topological and photocatalytic properties. The second one is dedicated to the discovery of novel physical phenomena, highlighting the breakdown of the phonon picture in heat transport in reduced dimension, and the emergence of novel hydrodynamic regimes.