COLLOQUIA

UNIVERSITY
OF TRENTO - Italy
Department of Physics

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Theory and Simulation of Materials, EPFL, and Laboratory for Materials Simulations, Paul Scherrer Institut

2023, February 15 – 2:00 p.m.
Room A103

To see a world in a grain of sand

Abstract

Electronic-structure simulations provide powerful capabilities to understand, predict, and design the properties and performance of novel materials and devices, and can nowadays support, streamline, and sometimes even inspire experimental efforts. I will discuss this research paradigm across the three themes of predictive accuracy, realistic complexity, and materials informatics.

First, I will argue how state-of-the-art functionals can capture not only challenging mixed-valence ground states but also charged excitations and spectroscopies. Then, I'll show how the quest to provide accurate microscopic descriptions of macroscopic properties can even inspire novel physical formulations, using examples taken from transport theories of solids. Last, I'll highlight how reliable and accurate simulations allow for systematic and even effortless explorations of materials space, enabling the discovery of novel materials with targeted properties.

These points underscore the bright future and opportunities arising from digitally-driven science, both for scientific discovery and technological innovation - not only improving at the speed of information-and-communication technologies, rather than of physical infrastructures, but also as a powerful and democratic instrument that can be shared worldwide at the flick of a button.

Further reading

N. Marzari, A. Ferretti, C. Wolverton, "*Electronic-structure methods for materials design*", Nature Materials, Vol. 20, June 2021 pp. 736-749
N. Mounet, M. Gibertini, P. Schwaller, D. Campi, A. Merkys, A. Marrazzo, T. Sohier, I. E. Castelli, A. Cepellotti, G. Pizzi & N. Marzari, "*Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds*", Nature Nanotechnology, 13, 2018, pp. 246–252

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