Department of Physics
Condensed Matter Physics
Clarendon Laboratory, Parks Road, Oxford OX1 3PU

UNIVERSITY OF OXFORD

CONDENSED MATTER PHYSICS COLLOQUIUM

Thursday 21 May at 14:30
Martin Wood Lecture Theatre, Department of Physics
(https://maps.app.goo.gl/WjG71uLF2D48n85B6)

Materials from first principles

Professor Nicola Marzari
University of Cambridge

Materials underpin many of the technologies that drive our economy and sustain our societies. Providing reliable, predictive descriptions of their behaviour from first principles remains a defining challenge for condensed-matter physics and materials science — one made increasingly urgent by the convergence of high-performance computing, machine learning, and artificial intelligence, which are transforming the scale and scope of materials design and discovery.

I will discuss recent progress along three directions. First, I will address predictive accuracy, focusing on functional theories of the spectral density to address electronic excitations and correlations.

Second, I will consider realistic complexity, introducing mesoscopic transport theories that bridge microscopic equations and macroscopic diffusion. Third, I will discuss materials informatics, emphasizing automation, agency, and autonomy in campaigns of materials discovery.

These ideas will be illustrated with three case studies: the Mott–Hubbard and charge-transfer regime of transition-metal monoxides; hydrodynamic heat transport in bulk compounds and micro-devices; and in charting the electronic structure of experimentally known inorganics, searching for novel properties and improved performance.

Host: Professor Marina Filip