EPFL Valais, ChE 602 Seminar, 22.12.2016

*Title: Adventures in Flatland*

**Abstract:**
"Understand, predict, and design" has been for a long time the informal mission statement of our group; since occasionally we do follow through on this, I'll take the chance to illustrate this paradigm with case studies taken from the burgeoning field of 2D materials. I'll discuss in particular the breakdown of the established but approximate picture of phonons being the heat carriers in crystals [1]; the engineering of Berry phases in nanostructures to create 1D electron and hole wires [2]; and our ongoing efforts to exfoliate all known 3D materials - this last made possible and straightforward by the development of our AiiDA materials' informatics platform [3].

[1] A. Cepellotti and N. Marzari, Thermal transport in crystals as a kinetic theory of relaxons, arXiv:1603.02608 (2016).

[2] M. Gibertini, G. Pizzi, N. Marzari, Engineering polar discontinuities in honeycomb lattices,Nature Communications 5, 5157 (2014); M. Gibertini and N. Marzari, Emergence of one-dimensional wires of free carriers in transition-metal dichalcogenides nanostructures, Nano Letters 15, 6229-38(2015).

[3] G. Pizzi et al., AiiDA: automated interactive infrastructure and database for computational science,Comp. Mat. Sci. 111, 218 (2016); http://aiida.net.

**Bio:**
Nicola Marzari holds a Laurea in physics from the University of Trieste (1992) and a PhD in physics from the University of Cambridge (1996). He was a NSF postdoctoral fellow at Rutgers University (1996-98) and a research scientist at the Naval Research Laboratory (1998-99) and at Princeton University (1999-01). In 2001 he was appointed assistant professor of computational materials science at the Massachusetts Institute of Technology, where he was promoted to associate professor in 2005 and to the Toyota Chair of Materials Engineering in 2009. In 2010 he joined the University of Oxford as its first Statutory Professor of Materials Modelling and director of the Materials Modelling Laboratory.
He moved to EPFL in 2011, as chair of Theory and Simulation of Materials; from 2014 he also directs the Swiss National Centre on Computational Design and Discovery of Novel Materials.