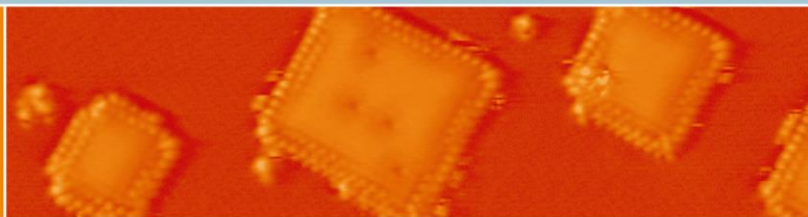




MARTIN-LUTHER-UNIVERSITÄT  
HALLE-WITTENBERG



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Time: 17:15 h  
Room: Conference Hall

Thursday,  
**January 25, 2018**

IAMO (Leibniz-Institut  
für Agrarentwicklung in  
Transformations-  
ökonomien)  
Theodor-Lieser-Str. 2  
06120 Halle

*There will be coffee from 17:00.*

**Prof. Nicola Marzari**

EPFL Lausanne, Switzerland

### **The power of not thinking: Materials' discovery in the 21<sup>st</sup> century**

Two-dimensional materials have seen in the past decade very dedicated experimental and theoretical efforts, in the quest for novel physics and functionalities. Here, we systematically explore with first-principles calculations all known inorganic materials, to identify those that could be exfoliated into two-dimensional layers. We start by curating experimental materials databases, collecting reliable data for 110,000 unique compounds. Then, we identify those that appear layered according to simple geometric and bonding criteria, and launch high-throughput calculations – based on van-der-Waals density-functional theory – to characterize binding energies, stability, and properties. Remarkably, we find 2000 inorganic compounds that can be exfoliated into novel two-dimensional materials, and recover in the process all known ones – from graphene to transition-metal dichalcogenides to boron nitride and black phosphorous.

I'll provide a perspective on the promising properties that we are uncovering – electronic, topological, optical – but will conclude on a more formal note, dedicated to the study of thermal transport in lower dimensions. Here, the great abundance of normal scattering processes leads to a hydrodynamic behaviour of the phonon gas, and to the failure of our common understanding of phonons being the individual carriers of heat.