UNIVERSITÄT DUISBURG ESSEN

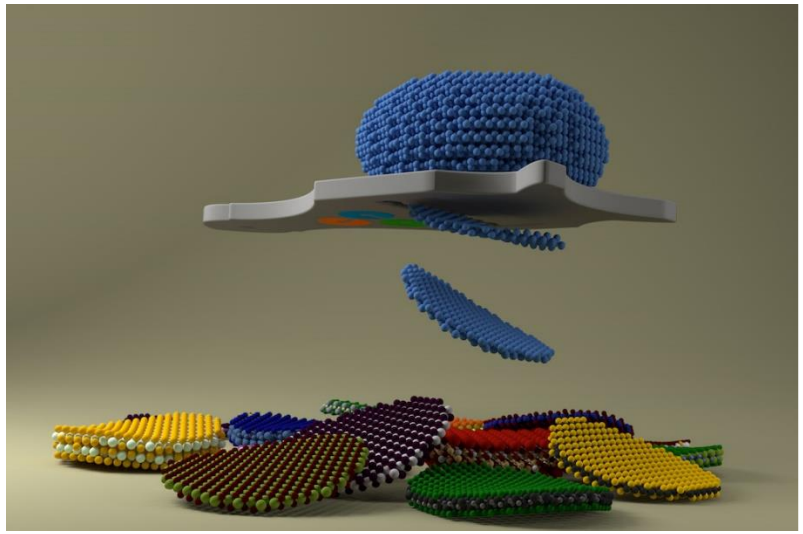
PHYSIK E=

Physikalisches Kolloquium

Mittwoch, 27.10.2021
13:00 Uhr
Hörsaal MC 122

The great acceleration in the design and discovery of novel materials

Prof. Dr. Nicola Marzari, École Polytechnique Fédérale de Lausanne



Materials are at the core of our technological advances, and are needed to address many of our societal challenges: from energy to information, from food to medicine. I'll highlight the great strides made in the last few years in the design and discovery of novel materials, where computational simulations can now precede, streamline, or accelerate experiments.
This acceleration is driven by the central paradigm of computational science (doubling performance every 14-16 months), combined with powerful and predictive quantum simulation techniques, and by the convergence of data mining and machine learning towards materials simulations. I'll also underscore the IT requirements needed to perform calculations in a reproducible, shareable, high-throughput mode.
A case study will be our computational exfoliation of all known inorganic materials, leading to ~3,500 promising candidates, for which I will discuss highlights for quantum spin Hall insulators, superconductors and spin FETs.