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ABSTRACT

Discovery and characterization of novel materials for electronic applications

We have performed an extensive high-throughput screening of known inorganic materials, in order to identify those that could be exfoliated into novel two-dimensional monolayers and multilayers [1], and could show promise for incorporation in novel electronic devices. The screening protocol first identifies bulk materials that appear layered according to a simple and robust chemical definition of bonding, determining then for all of these the binding energies of the respective monolayers, and their electronic state, magnetic configuration, and mechanical stability. Such protocol identifies a portfolio of close to 2,000 inorganic materials that appear either easily or potentially exfoliable, to be investigated further for promising properties. First focus has been on the the effective masses and mobilities (from the full solution of the Boltzmann transport equation); on topological invariants; and on superconductivity and charge-density waves. Thanks to the use of the AiiDA (http://aiida.net) materials' informatics platform, all the high-throughput calculations can be performed and streamlined in fully searchable and reproducible ways, they are stored in a database with their full provenance tree of all parent and children calculations, and can be shared with the community at large in the form of raw or curated data via the Materials Cloud (http://www.materialscloud.org) dissemination portal.

Reference:

1. Nicolas Mounet, Marco Gibertini, Philippe Schwaller, Davide Campi, Andrius Merkys, Antimo Marrazzo, Thibault Sohier, Ivano Eligio Castelli, Andrea Cepellotti, Giovanni Pizzi and Nicola Marzari, Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds, Nature Nanotechnology 13, 246–252 (2018).

BIO

Nicola Marzari holds the chair of Theory and Simulation of Materials at the École Polytechnique Fédérale de Lausanne, where he is also the director of the Swiss National Centre for Competence in Research NCCR MARVEL on Computational Design and Discovery of Novel Materials (a 12-year effort started in 2014 and involving more than 40 groups). Previous tenured appointments include the Toyota Chair for Materials Engineering at the Massachusetts Institute of Technology, and the first Statutory (University) Chair of Materials Modelling at the University of Oxford, where he was also the director of the Materials Modelling Laboratory. He is the current chairman of the Psi-k Charity and Board of

Trustees. More than 25 of his past group members hold faculty positions worldwide in the field, from Harvard to MIT, Imperial College, and Seoul National University.