



MAPEX COMMUNITY

U Bremen Excellence Chair

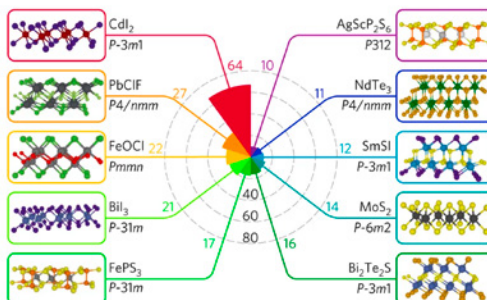
II NICOLA MARZARI – VISITING PROFESSOR 2019 – 2022

Nicola Marzari is one of the most prominent materials scientists in the world, as his nomination in the „Highly Cited Researcher 2018 List“ impressively proves. He holds the chair „Theory and Simulation of Materials (THEOS)“ at the EPFL in Lausanne (Switzerland), where he leads the MARVEL Center of Excellence for computational design and discovery of novel materials.

II THEORY AND SIMULATION OF MATERIALS @ EPFL

To understand, predict and design the properties of complex materials and devices from first-principles simulations is in the focus of the THEOS group. Its their research is dedicated to the development and application of computational modelling to outstanding problems in materials science, mainly using quantum-mechanical descriptions of interacting electrons and nuclei that are verified and validated against experimental results and higher-order theories. The computational laboratory allows to characterize or predict materials' properties directly from first-principles simulations, to screen or

design new materials and devices with high-throughput calculations and to connect microscopic and atomistic structure to macroscopic performance.



Left: Polar histogram showing the number of structures belonging to the ten most common 2D structural prototypes in the set of 1,036 easily exfoliable 2D materials. Mounet et al., Nature Nanotechnology 13, 246–252 (2018).

II NEW MATERIALS ON DEMAND @ UNIVERSITY OF BREMEN

Developing new materials on demand with the help of artificial intelligence, from the perspective of atoms, in a resource-saving and future-oriented way. The new U Bremen Excellence Chair, Prof. Nicola Marzari, and the scientists of MAPEX have set themselves this ambitious goal for the next four years.



Left: First visit of the U Bremen Excellence Chair, January 2019 (Andreas Breiter, Nicola Marzari, Lucio Colombi Ciacchi, Hanna Lührs)

While traditional material development requires elaborate and expensive experiments, Prof. Marzari's team uses a clever combination of physics-based and data-based modelling. „If we want to develop complex materials together with their synthesis and manufacturing processes on a high-performance computer, then we need realistic, physically sound models as well as new algorithms and computer science methods in order to generate material science knowledge from large amounts of data,“ says Marzari.

„The University of Bremen and its partner institutes on campus offer a unique combination of expertise in both modern materials science and artificial intelligence“ explains Prof. Lucio Colombi Ciacchi, current MAPEX spokesperson. „With the support of Nicola Marzari, we want to combine these existing competencies to break new ground in material and process development and, for the first time, to develop and to produce materials with individually tailored and locally varying thermo-chemo-mechanical properties.“

Students will also benefit greatly from the new holder of the excellence chair, who is very committed to teaching and has recently been awarded the title of ‚Best Teacher in Materials Science and Engineering‘ at EPFL. In addition to targeted lectures, Prof. Marzari wants to organize practical tutorials on materials informatics and address the general public about the importance of materials for society with an annual „Excellence Chair Lecture“.

II U BREMEN EXCELLENCE CHAIRS

The ‘U Bremen Excellence Chairs’ programme promotes the University of Bremen's internationalisation efforts on a high level. Eight Chairs will be supported for four to seven years by means of the so-called University Allowance funded within the Excellence Strategy.



Prof. Nicola Marzari

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