CENIDE & WIN Seminar Series on 2D-MATURE

DFG IRTG 2803 & NSERC CREATE

Miguel Marques

Ruhr-University Bochum

"Searching for novel binary and ternary 2D materials"

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10:00 a.m. ET / 16:00 p.m. CET

Miguel Marques received his PhD degree in Physics from the University of Würzburg in 2000, working under the supervision of E.K.U. Gross in the field of density functional theory for superconductors. He then held several post-doctoral positions in Spain, Germany, and in France. From 2005 to 2007 he was assistant professor at the University of Coimbra in Portugal. From 2007 to 2014 he was CNRS researcher at the University of Lyon 1, and from 2014 to 2023 professor at the Martin-Luther University of Halle-Wittenberg. He is now professor at the Research Center Future Energy Materials and Systems of the Ruhr University Bochum. His current research interests include density functional theory, superconductivity, application of machine learning to materials science, etc. He authored more than 200 articles, and has edited three books published by Springer in the Lecture Notes in Physics series. He also organized several summer schools and international workshops, such as the Benasque School and International Workshop in TDDFT, that takes place in Benasque, Spain every second year.

We present a symmetry-based systematic approach to explore the structural and compositional richness of two-dimensional materials. We use a combinatorial engine that constructs candidate compounds by occupying all possible Wyckoff positions for a certain space group with combinations of chemical elements. In this way we unveil an unprecedented variety of two-dimensional materials, covering the whole periodic table in more than 30 different stoichiometries. Among the discovered structures, we find examples that can be built by decorating nearly all Platonic and Archimedean tesselations as well as their dual Laves or Catalan tilings. We also obtain a rich, and unexpected, polymorphism for some specific compounds. We further accelerate the exploration of the chemical space of two-dimensional materials by employing machine-learning-accelerated prototype search, based on the structural types discovered in the systematic search. Finally, we present a couple of examples exhibiting interesting properties such as flat bands.