Max-Planck-Institut für
Struktur und Dynamik der Materie
Max Planck Institute for the Structure and Dynamics of Matter

IMPRS UFAST Call for PhD applications 2022/2023

IMPRS ULTRAFAST IMAGING & STRUCTURAL DYNAMICS

MR2- Exploiting extrapolative regimes of machine-learning algorithms for electronic structure properties of 2D materials

Title of PhD Project	**Exploiting extrapolative regimes of machine-learning algorithms for electronic structure properties of 2D materials**
Type	Theory
Supervisor(s)	Dr. Mariana Rossi, Prof. Lede Xian and Prof. Angel Rubio
Affiliation(s):	Max Planck Institute for the Structure and Dynamics of Matter
Number of positions:	1
Abstract:	2D materials have given rise to a fruitful search for emergent quantum properties of matter, based on intercalation of different 2D sheets and magic-angle alignments between sheets. The calculation of such properties in complex heterostructures or small-angle twisted-bilayers is hampered by the cost of simulation, related to the large size of such structures. In this project, we will apply and develop machine-learning techniques that are capable of learning the electronic structure [1]. The goal is the prediction of large-structure properties (band structures, optical spectra, etc.) at minimal computational cost but retaining ab initio quality and predictive power. Ultimately, the PhD candidate would build a database of structure-property relationships of these 2D materials and exploit in depth special regimes of twisted bilayer systems. Candidates with a background in physics or chemistry, with good math and programing skills are sought. We encourage the application of female candidates. [1] A. Lewis, A. Grisafi, M. Ceriotti, M. Rossi, *J. Chem. Theory Comput.* **17**, 7203–7214 (2021).
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