



IMPRS UFAST Call for PhD applications 2021/2022



Controlling phase transitions and electronic properties of TMDC-based Heterostructures

M. Rossi-1

Title of PhD Project	Controlling phase transitions and electronic properties of TMDC-based heterostructures.
Type	Theory
Supervisor(s)	Dr. Mariana Rossi
Affiliation(s):	Max Planck Institute for the Structure and Dynamics of Matter
Number of positions:	1
Abstract:	<p>The goal of this project is to unravel the physical origin of the temperature dependence of certain electronic properties of transition metal dichalcogenide (TMDC) interfaces (charge transfer, band gaps, dielectric properties, polarization) by disentangling electron-phonon coupling effects at a particular phase, from emerging properties related to different (potentially metastable) structural phases. In order to achieve this goal, the candidate will train machine-learned potentials based on highly accurate density-functional-theory energy evaluations and augment them with anisotropic many-body van der Waals dispersion terms. With such potentials, different phases can be explored by molecular dynamics in the isothermal-isobaric ensemble. In addition, the candidate will develop molecular-dynamics-based methods to drive phase transitions, as well as characterize the electronic properties of these phases.</p> <p>Candidates with a background in physics or chemistry, with good math and programming skills are sought. We encourage the application of female candidates. Collaborations with experimental groups will be part of the research program.</p>
Contact person for scientific questions about the project:	Mariana Rossi: mariana.rossi@mpsd.mpg.de