## 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 2024/2025



GB1 - Theory of Excitons, Charged Excitons and their Mutual Interactions in Moiré 2D Materials

Title of PhD Project	Theory of Excitons, Charged Excitons and their Mutual Interactions in
	Moiré 2D Materials
Туре	Theory
Supervisor(s)	Prof. Gabriel Bester
Affiliation(s):	Hamburg University
Number of positions:	1
Abstract:	The project aims to investigate the properties and interactions of excitons, charged excitons, and biexcitons in two-dimensional materials using advanced computational techniques. By leveraging a combination of Density Functional Theory (DFT) and screened configuration interaction methods, we will accurately calculate these excitonic properties with a focus on their optical properties. The candidate will utilize our state-of-the-art 2D-atomic effective pseudopotentials and recently developed force-field models to explore moiré structures comprising up to 10,000 atoms. These large-scale simulations will provide a comprehensive understanding of the electronic and optical properties of complex 2D heterostructures, where the twist angle enters as one of the key controlling parameters. The project offers an exciting opportunity to engage in cutting-edge research at the intersection of computational physics and material science, with many possible fruitful interactions with theory and experimental groups within IMPRS UFAST.
Contact person for	Prof. Gabriel Bester: gabriel.bester@uni-hamburg.de
scientific questions about	
the project:	
Research Group Website:	https://www.chemie.uni-
	hamburg.de/en/institute/pc/arbeitsgruppen/bester.html











International Max Planck Research School for Ultrafast Imaging & Structural Dynamics (IMPRS UFAST), Luruper Chaussee 149, Building 99, 22761 Hamburg, Germany Spokesperson: Prof. Dr. Angel Rubio, Coordinator: Dr. Neda Lotfiomran