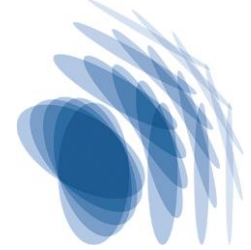


Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter



IMPRS UFAST Call for PhD applications 2025/2026



GB1 - Novel Ab-Initio Methodology for Trions and Biexcitons in Moiré and Janus 2D

Title of PhD Project	Novel Ab-Initio Methodology for Trions and Biexcitons in Moiré and Janus 2D Materials
Type	Theory
Supervisor(s)	Prof. Gabriel Bester
Affiliation(s):	Hamburg University
Number of positions:	1
Abstract:	<p>This PhD project focuses on the theoretical investigation of optical properties in 2D Moiré structures, Janus bilayers, and trilayers, with an emphasis on high-accuracy ab-initio predictions. Building on the innovative computational framework developed by the G. Bester group—based on screened configuration interaction, equivalent to the Bethe-Salpeter approach at the exciton level but extendable to trions and biexcitons—this work aims to elucidate complex many-particle excitations in large atomic systems. Recent advances by our group (e.g., "Beyond the K-valley: exploring unique trion states in indirect band gap monolayer WSe₂," npj 2D Materials and Applications, 2025) demonstrate the method's capacity to capture novel quasi-particle states with unprecedented accuracy.</p> <p>The candidate should have a solid background in solid-state or computational physics, and an enthusiasm for tackling fundamental questions through large-scale HPC computational techniques. This project offers an exciting opportunity for collaboration with experimental groups at IMPRS, including the new Mak and Shan directorates, as well as with renowned theorists such as the Angel Rubio group. Effective and open-minded communication are key advantages.</p>
Contact person for scientific questions about the project:	Prof. Gabriel Bester: gabriel.bester@uni-hamburg.de
Research Group Website:	https://www.chemie.uni-hamburg.de/en/institute/pc/arbeitsgruppen/bester.html

