

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

**MR1 – Non-adiabatic nuclear dynamics for charge excitations at
molecular/2D interfaces**



Title of PhD Project	Non-adiabatic nuclear dynamics for charge excitations at molecular/2D interfaces
Type	Theory
Supervisor(s)	Mariana Rossi
Affiliation(s):	Max Planck Institute for the Structure and Dynamics of Matter
Number of positions:	1
Abstract:	The candidate will develop methods based on TDDFT and multi-trajectory Ehrenfest dynamics, which capture non-perturbative nonadiabatic coupling in processes involving charge excitations at the interface of 2D confining materials and molecules or liquids. The goal is to will achieve a methodology that can account for quantum vibronic effects in weakly-bound systems with molecular components. A particular focus will lie on the study of “hybrid” vibrations that couple molecular liquids such as water with confining interfaces, aiming to elucidate effects such as the fast cooling of electronic degrees of freedom by water, following excitation.
Contact person for scientific questions about the project:	Mariana Rossi: mariana.rossi@mpsd.mpg.de
Research Group Website:	https://www.mpsd.mpg.de/research/groups/sabia

