



IMPRS UFAST Call for PhD applications 2026/2027

NR - Simulation of UV/x-ray attosecond pump probe interferometry for Analysis of coherent electronic wave packets in molecular crystals



Title of PhD Project	Simulation of UV/x-ray attosecond pump probe interferometry for analysis of coherent electronic wave packets in molecular crystals
Type	Theory
Supervisor(s)	Nina Rohringer
Affiliation(s):	UHH, DESY
Number of positions:	1
Abstract:	Attosecond UV pulses allow to create electronic wave packets in molecules. Thereby, electronic coherences result in additional forces on the nuclei, resulting in dynamics beyond the Born-Oppenheimer approximation and potentially enabling novel chemical reaction pathways. In our ERC-Synergy funded project we aim to study these electronic wave packets by time-resolved x-ray diffraction and spectroscopy. The successful candidate will develop a quantitative theory for transient x-ray absorption and x-ray interferometry. The project comprises the simulation of the electronic wave packets upon excitation with attosecond UV pulses with state-of-the-art quantum-chemistry methods. Subsequently, the time dependent x-ray refractive index will be determined, and predictions for interferometric measurement are made. The project will start for isolated small molecules. In a later phase, embedding techniques will be employed, to capture the time-dependent electronic structure of molecular crystals. These results will directly link to the time-resolved x-ray diffraction measurements. The project is in collaboration with the experimental groups of H. Chapman, S. Bajt and F. Calegry. We offer the opportunity to work in a multifaceted research project, that involves experiments at x-ray free electron laser sources worldwide.
Contact person for scientific questions about the project:	Nina Rohringer: nina.rohringer@desy.de
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