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

AR6 - Ab-initio nanoplasmonics, light shaping and light-induced dynamical correlations

Title of PhD Project	**Ab-initio nanoplasmonics, light shaping and light-induced dynamical correlations**
Type	Theory
Supervisor(s)	Prof. Angel Rubio, Dr. Franco Bonafe, Dr. Heiko Appel, Dr. Hannes Hübener, Dr. Carlos Bustamante
Affiliation(s):	Max Planck Institute for the Structure and Dynamics of Matter
Number of positions:	1
Abstract:	In this project, we are bringing together the research fields of ab-initio atomistic quantum dynamics and computational electrodynamics for a novel description of the nano-confinement of electromagnetic fields. This opens a vast set of novel applications in materials science, nano-plasmonics and spectroscopies. So far, exciting research has been done in these areas separately. The combination of these two dynamical methods in a fully-coupled way, will enable us to not only understand the role of the atomistic details of materials in the shaping of nano-confined light, but also to harness such spatiotemporally shaped fields to induce new properties in materials. Neither of the computational techniques developed so far have been able to tackle the full nature of some challenging open problems. Examples of such challenges are: computational design and optimization of photoelectron emission, and the impact of the field's shape and time-profile on electron tunneling or near-field enhanced spectroscopies, such as tip-enhanced Raman spectroscopy. The core method that will allow this is the new forward-backward coupled, self-consistent Maxwell-Kohn-Sham time-propagation scheme that has been recently implemented in the package Octopus [1,2]. The resulting predictions will be tested experimentally by our network of collaborators, giving rise to high-impact novel developments in several fields within nano-optics, high-resolution spectromicroscopies and near-field sensing. [1] https://octopus-code.org/wiki/Main_Page [2] R. Jestädt, M. Ruggenthaler, M. J. T. Oliveira, A. Rubio, & H. Appel, Advances in Physics, **68** (4), 225-333 (2019). DOI: 10.1080/00018732.2019.1695875
Contact person for scientific questions about the project:	Franco Bonafe: franco.bonafe@mpsd.mpg.de Heiko Appel: heiko.appel@mpsd.mpg.de Hannes Hübener: hannes.huebener@mpsd.mpg.de Angel Rubio: angel.rubio@mpsd.mpg.de Carlos Bustamante: carlos.bustamante@mpsd.mpg.de
Research Group Website:	https://theory.mpsd.mpg.de/