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 2020/2021

Maxwell-TDDFT nanoplasmonics and structured light shaping

A. Rubio-5

Title of PhD Project	**Maxwell-TDDFT nanoplasmonics and structured light shaping**
Type	Theory
Supervisor(s)	Dr. Franco Bonafe and Dr. Heiko Appel Prof. Angel Rubio
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 on one side and computational electrodynamics on the other side, to get a novel theoretical approach for the 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, either in ab-initio electron dynamics (such as time-dependent density functional theory, TDDFT) considering the external field as prescribed by an analytic expression, or in computational electrodynamics considering only approximations for the optoelectronic properties of matter. 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, such as the 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-TDDFT time-propagation scheme that has been recently implemented in the package Octopus. 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.
Contact person for scientific questions about the project:	Franco Paul Bonafe: franco.bonafe@mpsd.mpg.de Heiko Appel: heiko.appel@mpsd.mpg.de Angel Rubio: angel.rubio@mpsd.mpg.de