

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

AR4 – Polaritonic Chemistry in Plasmonic Cavities



Title of PhD Project	Polaritonic Chemistry in Plasmonic Cavities
Type	Theory
Supervisor(s)	Dr. Carlos Bustamante Dr. Franco Bonafé Dr. Heiko Appel Prof. Angel Rubio
Affiliation(s):	Max Planck Institute for the Structure and Dynamics of Matter
Number of positions:	1
Abstract:	This PhD will investigate how to <i>control chemical reactions with light</i> by studying molecules in plasmonic cavities under electronic and vibrational strong coupling. We use a new simulation framework that merges real-time solutions of Maxwell's equations for realistic cavity modes with quantum electron dynamics at the DFTB and DFT levels, enabling atomistic modeling of hundreds of molecules in experimentally relevant geometries. This approach reveals both collective and local molecular responses, and gives access to the spectral response of the full optical setup. This allows to study how number, arrangement, and orientation of molecules affect reactivity. By performing Ehrenfest and Born-Oppenheimer dynamics in setups with designed plasmonic nanostructures, we will study how cavity design can steer reaction pathways. The goal is to predict and tune reaction outcomes, in close collaboration with experimental partners, paving the way for a deeper, predictive understanding of polaritonic chemistry.
Contact person for scientific questions about the project:	Dr. Carlos Bustamante: carlos.bustamante@mpsd.mpg.de Dr. Franco Bonafé: franco.bonafe@mpsd.mpg.de Dr. Heiko Appel: heiko.appel@mpsd.mpg.de
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