## 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 2024/2025

**AR1-** Polaritonic Chemistry

Title of PhD Project

Number of positions:

Supervisor(s)

Affiliation(s):

Abstract:

Туре



PAFAST IMACING &

STRUCTURAL DYN
Polaritonic Chemistry
Theory
Prof. Angel Rubio, Dr. Dominik Sidler, Dr. Michael Ruggenthaler
Max Planck Institute for the Structure and Dynamics of Matter
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Seminal experimental results have demonstrated that molecules can be
strongly coupled to the (quantized) photon field of optical cavities. This can
induce dramatic chemical changes, which may eventually provide
unprecedented control of chemical reactions. Inspired by the early

experimental advancements, the field of *polaritonic chemistry* has recently emerged. Our group together with international collaborators has pioneered the first ab-initio methods, which are based on non-relativistic quantum electrodynamics. However, despite these significant advances, the relevant driving mechanisms of polaritonic chemistry remain an open theoretical question of utter relevance. To unravel the mysteries of polaritonic chemistry not only established concepts form quantum chemistry, and quantum optics need to be revisited, but recent theoretical evidence also suggests a fundamental theoretical connection to the physics of a spin glass. This novel aspect introduces the concept of frustration with spontaneous symmetry breaking in polaritonic chemistry, and it also brings it closer to the theory of solid-state physics.

All of which provides ideal ground to pursue cutting-edge interdisciplinary research. The PhD project can thus be tailored specifically to the background and interests of the applicant. It may involve fundamental theoretical questions, the development of novel algorithms and HPC code, as well as compelling applications.

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scientific questions about	Dr.Dominik Sidler: <u>dsidler@mpsd.mpg.de</u>
the project:	Dr. Michael Ruggenthaler: michael.ruggenthaler@mpsd.mpg.de
Research Group Website:	https://theory.mpsd.mpg.de/research/project/detail/qed_chemistry/







International Max Planck Research School for Ultrafast Imaging & Structural Dynamics (IMPRS UFAST), Luruper Chaussee 149, Building 99, 22761 Hamburg, Germany Spokesperson: Prof. Dr. Angel Rubio, Coordinator: Dr. Neda Lotfiomran



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