

# 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 2021/2022



**Polaritonic Chemistry**

**A. Rubio-8**

<b>Title of PhD Project</b>	<b>Polaritonic Chemistry</b>
<b>Type</b>	Theory
<b>Supervisor(s)</b>	Dr. Michael Ruggenthaler, Dr. Franco Bonafe, and Dr. Heiko Appel Prof. Angel Rubio
<b>Affiliation(s)</b>	Max Planck Institute for the Structure and Dynamics of Matter
<b>Number of positions:</b>	1
<b>Abstract:</b>	<p>Based on seminal experimental results, which highlight that coupling molecules strongly to the photon field of an optical cavity can lead to dramatic changes of, e.g., chemical reactions, the new interdisciplinary field of polaritonic chemistry has emerged. This field inherits its name from the appearance of light-matter hybrid states, which are termed polaritons.</p> <p>Our group together with international collaborators has developed the first ab-initio methods, which are based on non-relativistic quantum electrodynamics, for polaritonic chemistry, These methods (e.g. quantum-electrodynamical density-functional theory) have by now provided novel and critical insight into the basic principles of how the quantized electromagnetic field can change chemistry.</p> <p>In this project these numerical methods are to be further developed and used to gain deeper understanding of cavity-modified chemistry and to predict novel effects due to strong light-matter coupling. A focus is on the connection between collective and single-molecule strong coupling as well as on the impact of realistic (lossy multi-mode) cavities and the construction of phenomenological models based on ab-initio results to rationalize these findings.</p>
<b>Contact person for scientific questions about the project:</b>	Michael Ruggenthaler: <a href="mailto:michael.ruggenthaler@mpsd.mpg.de">michael.ruggenthaler@mpsd.mpg.de</a> Franco Paul Bonafe: <a href="mailto:franco.bonafe@mpsd.mpg.de">franco.bonafe@mpsd.mpg.de</a> Heiko Appel: <a href="mailto:heiko.appel@mpsd.mpg.de">heiko.appel@mpsd.mpg.de</a> Angel Rubio: <a href="mailto:angel.rubio@mpsd.mpg.de">angel.rubio@mpsd.mpg.de</a>

