

# 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 2022/2023



MR1- Theoretical modelling of light-driven nuclear motion

<b>Title of PhD Project</b>	<b>Theoretical modelling of light-driven nuclear motion</b>
<b>Type</b>	Theory
<b>Supervisor(s)</b>	Dr. Mariana Rossi
<b>Affiliation(s):</b>	Max Planck Institute for the Structure and Dynamics of Matter
<b>Number of positions:</b>	1
<b>Abstract:</b>	<p>The relationship between atomic structure and electronic, optical, and mechanical properties in condensed-phase systems is a subject of intense research, despite its long history. In particular, novel methods to control the structure of a solids and confined matter with exquisite precision and in a reversible manner by exploiting light-matter coupling, can open space for the design of new technological paradigms. This project will focus on the advancement of theoretical modeling of THz light-induced structural dynamics - an area that needs more attention as the complexity of the materials that are addressed increase. The student will help the development of novel and predictive ab-initio frameworks by joining many-body perturbative methods and advanced molecular-dynamics techniques, with calculations based on density-functional theory and machine-learned potentials.</p> <p>Candidates with a background in physics or chemistry, with good math and programing skills are sought. We encourage the application of female candidates. Collaborations with the group of Prof. Fabio Caruso (Uni. Kiel) and experimental partners will be part of the research program.</p>
<b>Contact person for scientific questions about the project:</b>	<a href="mailto:mariana.rossi@mpsd.mpg.de">mariana.rossi@mpsd.mpg.de</a>

