



IMPRS UFAST Call for PhD applications 2020/2021



Water at interfaces: Nuclear quantum effects in and out of equilibrium

M. Rossi

Title of PhD Project	Water at interfaces: Nuclear quantum effects in and out of equilibrium
Type	Theory
Supervisor(s)	Dr. Mariana Rossi
Affiliation(s):	Max Planck Institute for the Structure and Dynamics of Matter
Number of positions:	1
Abstract:	<p>The microscopic characterization of water at interfaces is a key problem in many areas of science. Two effects that are rarely addressed in simulations, namely nuclear quantum effects and applied bias voltages can strongly impact the atomic and electronic structure of water in contact with solid surfaces. Describing the interplay of these two effects requires joining theoretical techniques such as density-functional theory, non-equilibrium Green's functions, and the path integral formulation of quantum mechanics. Such a framework would allow the characterization of the dynamical structure of the interface and the simulation vibrational spectroscopy techniques that can be directly compared to cutting edge experiments.</p> <p>In this project, the candidate will have the opportunity of developing theories that set the formulation of path integral techniques in non-equilibrium steady states on a solid ground. They will also employ these theories within atomistic simulations that will unveil the mechanisms of surface-catalyzed water dissociation in and out of equilibrium and with time resolution. A connection to experiment will be ensured through the simulation of different flavors of vibrational sum-frequency generation in these ensembles.</p> <p>Candidates with a background in physics or chemistry, with good math and programming skills are sought. Collaborations with experimental groups will be part of the research program.</p>
Contact person for scientific questions about the project:	Mariana Rossi: mariana.rossi@mpsd.mpg.de Alan Lewis: alan.lewis@mpsd.mpg.de