



IMPRS UFAST Call for PhD applications 2021/2022



New approximations to quantum dynamics for vibrational spectroscopy of high-dimensional systems

M. Rossi-2

Title of PhD Project	New approximations to quantum dynamics for vibrational spectroscopy of high-dimensional systems
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>An effective way to characterize the structure of complex systems is through vibrational spectroscopy. Within linear response theory, these spectroscopies can be related to expressions involving time correlation functions of different interactions of the electronic density with electric fields, like dipole moments or polarizability tensors. The impact of nuclear quantum effects in these quantities can be dramatic, but their calculation for systems with hundreds of degrees of freedom is very challenging. While much improvement has been achieved within <i>ad hoc</i> methodologies like thermostatted ring polymer molecular dynamics (TRPMD), in many situations a more rigorous treatment is necessary. In this project, the candidate will devise new approximations based on generalized Langevin equations derived from more rigorous quantum dynamics methods, as well as exploit analytical continuation techniques with Bayesian-inference-based regularization forms.</p> <p>Candidates with a background in physics or chemistry, with very good math and programming skills are sought. We encourage the application of female candidates.</p>
Contact person for scientific questions about the project:	Mariana Rossi: mariana.rossi@mpsd.mpg.de