



IMPRS UFAST Call for PhD applications 2020/2021



Ab initio dynamical correlations and their spectroscopic fingerprints in 2D quantum materials

M. Sentef-3

Title of PhD Project	Ab initio dynamical correlations and their spectroscopic fingerprints in 2D quantum materials
Type	Theory
Supervisor(s)	Dr. Michael Sentef
Affiliation(s):	Max Planck Institute for the Structure and Dynamics of Matter
Number of positions:	1
Abstract:	<p>The intersection between ultrafast materials science and strongly correlated systems has provided new beyond-equilibrium insights into the interplay between lattice, charge, spin, and orbital degrees of freedom [1]. One important aspect concerns the role of model parameters, such as Hubbard U, in the short-time dynamics. We have recently predicted a dynamical modulation of U in a laser-driven charge-transfer insulator [2] based on time-dependent density functional theory calculations. A related effect was measured experimentally in a correlated Weyl semimetal [3]. This project aims at a more detailed microscopic understanding of dynamical correlations in 2D materials. The PhD candidate will learn nonequilibrium methods for correlated many-body systems (nonequilibrium Green's functions, time-dependent density functional theory) and apply them to selected model systems. The goal is to gain a detailed understanding of the role of electronic excitations as well as the coupling to the crystal lattice, which has recently been suggested to lead to photo-molecular superconductivity in an experimental-theoretical collaboration [4], for such dynamical correlation effects. The candidate will be embedded in an international highly collaborative research team with theorists as well as experimentalists working on the frontier of ultrafast material science.</p> <p>[1] S. Gerber et al., Science 357, 71 (2017) [2] N. Tancogne-Dejean, M. A. Sentef, A. Rubio, PRL 121, 097402 (2018) [3] S. Beaulieu et al., arXiv:2003.04059 [4] M. Buzzi et al., PRX 10, 031028 (2020)</p>
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