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

HS1- Singlet exciton fission in organic molecular crystals

Title of PhD Project	**Singlet exciton fission in organic molecular crystals -- ultrafast structural and electronic dynamics**
Type	Experimental
Supervisor(s)	Dr. Heinrich Schwoerer Dr. Sascha Epp, Dr. Gabriele Tauscher
Affiliation(s):	Max Planck Institute for the Structure and Dynamics of Matter
Number of positions:	1
Abstract:	Singlet Exciton Fission in organic molecular solids, the spontaneous splitting of one singlet exciton into two triplet excitons, conceptionally enables an increase of photovoltaic efficiency. A beneficial technical implementation of this concept, however, requires a thorough understanding of exciton dynamics and correlations in organic solids, which are determined by molecular orbital shapes, symmetries, overlaps and population. In particular, structural intra- and inter-molecular (lattice) motions, triggered by the photo excitation, severly influence fission yields by modulating long reaching electronic correlations. In this project we study polyacene single crystals, an ideal set of model systems for singlet exciton fission, with our new combined femtosecond transient absorption and ultrafast electron diffraction machine, equipped with cryo-cooling down to 20 K. With these complementary experimental approaches, it allows systematic investigation of both, electronic and structural dynamics on time and spatial scales relevant for the singlet fission process. The PhD project entails all aspects of this endeavor, from sample preparation with an ultramicrotome, femtosecond laser operation, electron diffractometry, spectroscopy, data analysis, physics and chemistry of organic solids; and thereby provides the opportunity for a broad and throrough scientific and technological training in a small team of experienced "ultrafast scientists". Lit.: Seiler, Schwoerer et al. Sci. Adv. **7**, eabg0869 (2021).
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