O 32: Topical Talk Witte

Time: Tuesday 9:30–10:15 Location: TRE/PHYS

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Excitons in molecular solids: from unitary films to donor-acceptor co-crystals — •Gregor Witte — Renthof 7, 35032 Marburg

Their strong light-matter interaction makes organic semiconductors (OSCs) promising candidates for optoelectronic devices. However, the microscopic picture of photophysical excitations and their properties is still incomplete. Reasons for this are the different nature of excitons in inorganic and organic SCs and the frequently used simplified description of excitons in OSCs within the framework of H- and J-aggregates, which disregards high-energy states and the delocalization of wave functions. Optical transmission-absorption measurements on single crystals or films with large crystalline domains enable the spectroscopy of higher energy excitons and, by means of polarization- and direction-resolved measurements, also a correlation with the molecular packing motif. Among OSCs, acenes represent an ideal platform for exciton studies, as they allow both polymorph-selective crystallization and versatile modification of the molecular electronic structure through chemical substitutions. Furthermore, also highly ordered acene-perfluoroacene cocrystals can be produced, which enable detailed characterizations of heteromolecular charge transfer excitons in molecular donor-acceptor systems with well-defined internal interfaces. In this talk I will present some of our recent exciton studies on various acenes, which combine polarization-resolved optical spectroscopy with modern ab initio calculations based on density functional theory and many-body perturbation theory.