SYET 1: Symposium on Exciton Transfer in Ordered Atomic and Molecular Structures

Time: Thursday 10:30–12:30 Location: SPA Kapelle

Invited Talk SYET 1.1 Thu 10:30 SPA Kapelle

On the role of charge transfer excitations in mediating triplet diffusion, singlet fission and dissociation in organics — •David Beljonne — Chimie des Matériaux Nouveaux & Centre d'Innovation et de Recherche en Matériaux Polymères, Université de Mons, Belgium

Primary photoexcitations in organic materials are strongly bound singlet Frenkel-like excitons coupled to a local lattice reorganization (polaronic excitons). In some molecular crystals such as oligoacenes, singlet excitons undergo an efficient spin-conserving fission process yielding two triplet excitons. Besides being of interest from a fundamental point of view, this process opens new opportunities to break the Schockley-Queisser limit in single junction organic solar cells. Singlet fission has thus retained lots of attention recently. We will review some recent works done in our lab and elsewhere on the fundamentals of singlet fission and point in particular to the importance of charge-transfer excitations in mediating the process, through either admixture of charge-transfer character into the lowest exciton states or via a super-exchange mechanism. The same effects also affect the rates and diffusion coefficients of the resulting triplets. We will present a first-principle study of triplet transport in an organic crystal taking into account such effects in addition to thermally activated crystal phonons and molecular vibrations. Finally, if time permits, a brief discussion of the mechanisms by which bound polaron pairs can escape from their Coulomb attractive well will be presented and analyzed in the light of recent experimental results.

Invited Talk SYET 1.2 Thu 11:00 SPA Kapelle

Disorder engineered long-range exciton migration in J-aggregates - observation of fluorescence from low-laying individual Lévy states — •Ivan Scheblykin[1], Aboma Merdasa[1], Ángel Jiménez[2], Theo Kaiser[2], and Frank Würthner[2] — [1]Chemical Physics, Lund University, PO Box 124, 22100 Lund, Sweden — [2]Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Fluorescence microscopy enables us to observe fluorescence of individual 1D J-aggregates of PBI dyes.[2] Single J-aggregate spectroscopy and super-resolution microscopy at 77K revealed formation of "outliers"-exciton states situated much lower than the "normal" exciton band edge.[3] It is the specific properties of the environment that lead to Lévy statistics of the energetic disorder in J-aggregates characterized by a heavy low-energy tail. The emission of the outlier appeared as a blinking band at the red tail of the temporally stable (non-blinking) main exciton fluorescence band. In addition the spatial localization of the red-band emission was tens of nanometers different from that of the main exciton emission. We attribute the observed phenomena to efficient exciton funneling through the entire 1D aggregate composed of hundreds of molecules to a single outlying exciton state acting as a trap. [1] I.G. Scheblykin, et al J.Phys.Chem.B 105(2001)4636. [2] H.Z. Lin et al, Nano Letters 10(2010)620. [3] A. Eisfeld et al, Phys.Rev.Lett.105(2010)137402.

Invited Talk SYET 1.3 Thu 11:30 SPA Kapelle

Quantum dynamics of molecular and atomic aggregates — •Alexander Eisfeld — MPI PKS Dresden

I will give an introduction into the topic, focusing on the similarities and differences between molecular and Rydberg aggregates.

Then I will present recent results on the entanglement dynamics of Rydberg aggregates.

Invited Talk SYET 1.4 Thu 12:00 SPA Kapelle

Energy transport in ultracold Rydberg aggregates — •Matthias Weidemüller — Physikalisches Institut, Universität Heidelberg, Germany

Highly excited atoms (Rydberg atoms) can serve as a model system to study energy transport under well controlled conditions [1]. I will give an overview over the latest developments and prospects of this field. In particular, recent results on *in-situ* imaging of the dynamics of dipole-mediated energy transport in an ultracold Rydberg gas will be presented [2].

[1] T.F. Gallagher and P. Pillet, Adv. At. Mol. Opt. Phys. **56**, 161 (2008).

[2] G. Günter *et al.*, Science **342**, 954 (2013).