

## CPP 6: Electronic and Optical Properties of Organic Systems I

Time: Monday 11:30–12:45

Location: H39

**Topical Talk**

CPP 6.1 Mon 11:30 H39

**Triplet exciton diffusion in organic semiconductors** — •ANNA KÖHLER — Department of Physics, University of Bayreuth, Bayreuth, Germany

Efficient triplet exciton emission has allowed improved operation of organic light-emitting diodes (LEDs). To enhance the device performance, it is necessary to understand what governs the motion of triplet excitons through the organic semiconductor. We use a series of poly(p-phenylene)-type conjugated polymers and oligomers of variable degree of molecular distortion (i.e. polaron formation) and energetic disorder as model systems to study the Dexter-type triplet exciton diffusion in thin films. We show that triplet diffusion can be quantitatively described in the framework of a Holstein small polaron model (Marcus theory) that is extended to include contributions from energetic disorder. The model predicts a tunnelling process at low temperatures followed by a thermally activated hopping process above a transition temperature. In contrast to charge transfer, the activation energy required for triplet exciton transfer can be deduced from the optical spectra. We discuss the implications for device architecture.

CPP 6.2 Mon 12:00 H39

**Selective excitation of exciton transitions in PTCDA crystals and films** — •REINHARD SCHOLZ<sup>1</sup>, LINUS GISSLEN<sup>1</sup>, VENKAT R. GANGILENKA<sup>2</sup>, LYUBOV V. TITOVA<sup>2</sup>, LEIGH M. SMITH<sup>2</sup>, L. A. AJITH DE SILVA<sup>3</sup>, and HANS-PETER WAGNER<sup>2</sup> — <sup>1</sup>Walter Schottky Institut, Technische Universität München — <sup>2</sup>Department of Physics, University of Cincinnati — <sup>3</sup>Department of Physics and Geology, Northern Kentucky University

Photoluminescence excitation studies on 3,4,9,10-perylene tetracarboxylic dianhydride (PTCDA) single crystals and polycrystalline PTCDA films are compared to the calculated excitonic dispersion deduced from an exciton model including the coupling between Frenkel excitons and charge transfer (CT) along the stacking direction. For excitation energies below the 0-0 Frenkel exciton absorption band at 5 K, these measurements enable the selective excitation of several CT states. The CT2 state involving stacked PTCDA molecules gives an excitation resonance for photoluminescence from the self-trapped CT2 exciton and from the non-relaxed CT2-nr state. Moreover, the fundamental transition of the CT1 involving both basis molecules in the crystal unit cell can be determined from the respective excitation resonance. The excitation energy dependence of the different emission bands allows the assignment of the fundamental transition energies of the CT2 and CT1 excitons to 1.95 eV and 1.98 eV, respectively. When the excitation energy exceeds 2.10 eV, we observe a dominating emission channel related to the indirect minimum of the lowest dispersion branch dominated by Frenkel excitons.

CPP 6.3 Mon 12:15 H39

**A new dimension in controlling ultrafast exciton dynamics of mesoscopic chromophore aggregates by fractal geometry** — •DMITRI V. VORONINE — Institut für Physikalische Chemie, Universität Würzburg, Würzburg, Germany

Ultrafast exciton percolation dynamics in mesoscopic chromophore aggregates was investigated using femtosecond transient absorption spectrometry. Ultrashort laser pulse excitation resulted in exciton-exciton annihilation whose rate depends on the spectral dimension of inhomogeneously broadened aggregates. The value of the spectral dimension and, therefore, the geometry of exciton percolation pathways can be controlled by varying the fractal aggregate geometry which is characterized by the fractal dimension. The fractal geometry dependence was shown for two types of porphyrin homo-aggregates: cationic (Pagg) and anionic (TPPS) porphyrins. The possibility to control the fractal and spectral dimensions of a porphyrin hetero-aggregate was also investigated. These results might be useful for the design of new materials for artificial light harvesting applications and for a better understanding of exciton dynamics in analogous systems such as conjugated polymers, carbon nanotubes, and others.

CPP 6.4 Mon 12:30 H39

**Absorption and Emission Spectroscopic Characterisation of 8-Amino-Riboflavin** — •AMIT TYAGI<sup>1</sup>, PEYMAN ZIRAK<sup>1</sup>, ALFONS PENZKOFER<sup>1</sup>, TILO MATHES<sup>2</sup>, PETER HEGEMANN<sup>2</sup>, MATTHIAS MACK<sup>3</sup>, and SANDRO GHISLA<sup>4</sup> — <sup>1</sup>Institut II - Experimentelle und Angewandte Physik, Universität Regensburg, Universitätsstr. 31, 93053 Regensburg — <sup>2</sup>Institut für Biologie / Experimentelle Biophysik, Humboldt Universität zu Berlin, Invalidenstr. 42, 10115 Berlin — <sup>3</sup>Institut für Technische Mikrobiologie, Hochschule Mannheim, Paul-Wittsack-Str. 10, 68163 Mannheim — <sup>4</sup>Universität Konstanz, Fakultät für Biologie, Postfach 5560 M644, 78457 Konstanz

The flavin dye 8-amino-8-demethyl-D-riboflavin (AF) in the solvents water, DMSO, and methanol was studied by absorption and fluorescence spectroscopy. The first absorption band is red-shifted compared to riboflavin, and blue-shifted compared to roseoflavin. The fluorescence quantum yields are 0.22 for AF in water, 0.37 for AF in methanol, and 0.50 for AF in DMSO. The fluorescence lifetimes were found to be 2.3 ns in water, 4.9 ns in methanol, and 5.1 ns in DMSO. The non-radiative decay is thought to be dominated by internal conversion and intersystem crossing. The photo-stability of AF was studied by prolonged light exposure. For blue-light exposure (425-500 nm) quantum yields of photo-degradations were determined to be 0.000018 for AF in water and methanol, and 0.000089 for AF in DMSO. The main degradation product of AF was found to be 8-amino-lumichrome (AL, absorption rise in 310-380 nm region). AF in DMSO additionally degraded to 8-aminoflavin quinine-methide tautomer.