

## CPP 12: Poster: Electronic and Optical Properties of Organic Systems

Time: Monday 16:30–18:00

Location: Poster C

CPP 12.1 Mon 16:30 Poster C

**Photo-Induced Phase Changes in Azobenzene-Containing Materials** — ●HUBERT AUDORFF<sup>1</sup>, LOTHAR KADOR<sup>1</sup>, ROLAND WALKER<sup>2</sup>, and HANS-WERNER SCHMIDT<sup>2</sup> — <sup>1</sup>University of Bayreuth, Institute of Physics and BIMF, D-95440 Bayreuth, Germany — <sup>2</sup>University of Bayreuth, Macromolecular Chemistry I and BIMF, D-95440 Bayreuth, Germany

The photo-induced formation of liquid-crystalline phases in azobenzene-containing amorphous materials is demonstrated. Liquid-crystalline polymers and low-molecular-weight glass formers can be quenched into a stable amorphous phase at room temperature. During the inscription of holographic intensity gratings, the illuminated areas become liquid-crystalline, which stabilizes the orientation of the azobenzene units, leading to stable gratings. Another advantage of the quenched polymeric materials is that the writing times are shorter by several orders of magnitude as compared to liquid-crystalline azobenzene compounds. With a series of low-molecular-weight tris-azobenzene derivatives, a remarkably stable light-induced orientation of the chromophores in initially amorphous thin-film architectures is demonstrated for the first time. The liquid-crystalline character is caused by spacers between the tris-functionalized benzene core and the three azobenzene moieties as well as polar end groups. The formation of the liquid-crystalline phase manifests itself in a pronounced post-development of the inscribed ratings, *i. e.*, an increase of the diffraction efficiency after the end of the writing process.

CPP 12.2 Mon 16:30 Poster C

**Frequency-Domain FLIM Measurements of Fluorophore Mixtures with a Custom-Built Low-Cost Setup** — ●THOMAS BEZOLD and LOTHAR KADOR — University of Bayreuth, Institute of Physics and Bayreuther Institut für Makromolekülforschung (BIMF), 95440 Bayreuth, Germany

Fluorescence lifetime imaging microscopy (FLIM) in the frequency domain is applied to different binary mixtures of fluorophores. The custom-built setup is based on a confocal microscope and employs standard communications-type radiofrequency electronics. Excitation is performed with a cw laser which is amplitude-modulated with an acousto-optic modulator (AOM). Modulation frequencies between 25 and 50 MHz are generated with a computer-controlled direct digital synthesizer (DDS). The fluorescence signal of the sample is demodulated at the fixed frequency of 70 MHz with an I-Q demodulator. Its modulation amplitude and phase shift with respect to the excitation yield information about the fluorescence lifetime(s) in the sample. Single- and bi-exponential fluorescence decays are analysed with a polar-plot technique [1].

[1] G. I. Redford and R. M. Clegg, *J. Fluor.* **15**, 805 (2005).

CPP 12.3 Mon 16:30 Poster C

**Soft x-ray dichroism to explore the molecular orientation using scanning x-ray transmission microspectroscopy (STXM)** — ●STEPHAN WENZEL, ANDREAS SPÄTH, CHRISTIAN HUB, and RAINER H. FINK — ICMM, Univ. Erlangen, Egerlandstraße 3, 91058 Erlangen, Germany

Scanning transmission soft X-ray microspectroscopy (STXM) has proven excellent spatial resolution (< 20 nm) in combination with spectroscopic information to investigate ultrathin samples. The superior information relies on the photon-energy specific absorption which offers high elemental and chemical contrast. Soft x-ray linear dichroism is established to analyze the molecular orientations in thin film or bulk samples from the angle-dependant absorption. In conventional STXM, the incident angle is fixed by the microscopy geometry. We demonstrate how a rotational device can be used to derive the molecular orientations in organic nano- and microcrystals. We present microspectroscopic studies of TCNQ, NTCDA and NDCI-nanocrystals prepared on commercial Si3N4 membranes. We compare the derived structures from different spectral analysis routines, *i.e.* stack analysis of images and from line scans. The work is funded by the BMBF under contract 05KS7WE1.

CPP 12.4 Mon 16:30 Poster C

**Optical analysis of trap states in amorphous organic semiconductor films** — ●HARALD GRAAF<sup>1</sup>, FRANK FRIEDRISZK<sup>1,2</sup>, and

CHRISTIAN VON BORCZYKOWSKI<sup>1</sup> — <sup>1</sup>Center of nanostructured Materials and Analytics, Chemnitz University of Technology, 09126 Chemnitz, Germany — <sup>2</sup>Institut für Physik, Universität Rostock, 18051 Rostock, Germany

Increasing interest is drawn on thin organic semiconductor films in opto-electronic devices. While for applications like field-effect transistors and photovoltaic cells highly ordered morphologies resulting in higher charge carrier mobilities are requested, for other purposes like organic light emitting diodes amorphous arrangement of the molecules is needed. Here lower mobilities increase the recombination rate leading to a higher photon yield. In such systems trap states can influence dramatically the luminescence in its intensity and spectral regime.

We will show recent results on amorphous films of a perylene dye with a rather high concentration of trap states. These trap states act as sinks for the excitons and leads therefore to a clear shift of the luminescence to the red compared to the monomer emission. Temperature depended and time resolved measurements give a clear hint for the population of the traps from the exciton band. Comparisons with previous electrical measurements lead us to the assumption, that these traps are also dominating the charge carrier mobility within the material.

CPP 12.5 Mon 16:30 Poster C

**Enwrapping of tubular J-aggregates using dye-labeled polyelectrolytes** — ●OMAR AL-KHATIB<sup>1,2</sup>, HELMUTH MÖHWALD<sup>1</sup>, JÜRGEN P. RABE<sup>2</sup>, CHRISTOPH BÖTTCHER<sup>3</sup>, and STEFAN KIRSTEIN<sup>2</sup> — <sup>1</sup>Max-Planck-Institute of Colloids and Interfaces, Potsdam, Germany — <sup>2</sup>Humboldt University Berlin, Department of Physics, Germany — <sup>3</sup>Freie Universität Berlin, Researchcenter for Electron Microscopy, Germany

In this contribution we demonstrate the coating of tubular J-aggregates with dye-labeled polyelectrolytes. The tubular J-aggregates are formed by an amphiphilic cyanine dye in aqueous solutions [1]. Due to the amphiphilic character of the molecules their aggregates possess a negatively charged surface, which can be utilized for the adsorption of oppositely charged polyelectrolytes. Poly(diallyldimethylammonium chloride) (PDAC) and poly(allylamine hydrochloride) (PAH) labeled with different fluorescent dyes may act as donors or acceptors within a Förster energy transfer (FRET) process.

The enwrapping is verified by cryogenic transmission electron microscopy (cryo-TEM). The FRET is investigated by means of optical absorption and fluorescence spectroscopy. These experiments provide evidence for energy transfer between the aggregate and the dye-labeled polyelectrolyte shell.

[1] S.Kirstein, S. Dähne, *International Journal of Photoenergy*, Volume 2006, Article ID 20363, 1-21

CPP 12.6 Mon 16:30 Poster C

**Spectroscopic and Theoretical Investigations on Pd(II) and Pt(II) Dithiocarbamates** — ●R. WENISCH<sup>1</sup>, D. FÖRRER<sup>2</sup>, S. GROSS<sup>2</sup>, M. CASARIN<sup>2</sup>, D. MONTAGNER<sup>2</sup>, A. VITTADINI<sup>2</sup>, M. HELM<sup>1</sup>, E. TONDELLO<sup>2</sup>, and S. GEMMING<sup>1</sup> — <sup>1</sup>FZ Dresden-Rossendorf, Dresden, Germany — <sup>2</sup>Dept. of Chemistry Univ. Padua, Padua, Italy

In coordination chemistry, the nature and strength of the metal-ligand interaction has attracted much interest. Metal-sulfur complexes, in particular in comparison with their oxygen-based analogues, are intriguing as the sulfur atoms are polarized more easily. The use of specifically tailored sulfur-based ligands allows for tuning the complex functional properties. Among them, electronic properties are very sensitive to changes in the sulfur coordination sphere, suggesting potential uses as molecular switches in optoelectronic devices. Metal dithiocarbamates [R<sub>2</sub>NCS<sub>2</sub>]<sub>2</sub>M have been extensively studied by IR and UV-vis. spectroscopy, ESR and to a limited extent XPS and UPS. Here, we present experimental and theoretical studies investigating the electronic properties of a series of dithiocarbamates of Pd(II) and Pt(II): the pyrrolidine-based one and the 1-pyrrolidinecarbodithioate methyl ester (PyDTM). MX<sub>2</sub>(PyDTM) (M = Pt/Pd; X = Cl/Br) were analyzed by XPS and by FT-IR spectroscopy. DFT calculations yielded details on the electronic structure and allowed for unambiguous assignment of the IR spectral features. Ionization energies were evaluated with the asymptotically correct LB94 potential and the two components ZORA.

CPP 12.7 Mon 16:30 Poster C

**Coupling of Frenkel excitons, charge transfer excitons and vibrations in linear absorption spectra of polyacene crystals**— IVAN LALOV<sup>1,2</sup>, ●CHRISTOPH WARNS<sup>2</sup>, and PETER REINEKER<sup>2</sup> —  
<sup>1</sup>Faculty of Physics, Sofia University, Sofia 1164, Bulgaria — <sup>2</sup>Institute for Theoretical Physics, Ulm University, 89069 Ulm, Germany

The linear absorption spectra of the crystals of anthracene, tetracene, and pentacene have been calculated in the case of coupling between Frenkel excitons (FEs), charge transfer excitons (CTEs) and intramolecular vibrations. The models and their parametrization for FEs and CTEs in the  $(a, b)$  plane of those crystals, first developed by P. Petelenz et al., have been used in the numerical simulations of the linear absorption.

The calculated excitonic and vibronic spectra allow to draw two main conclusions. First, CTEs and their vibronics will manifest themselves in linear absorption of light polarized along the monoclinic axis only (i.e. for tetracene and pentacene along the crystallographic  $b$ -axis). Second, the vibronic coupling (FE-phonon and CTEs-phonon) emphasizes and increases the number of the maxima of CTEs manifested in the linear absorption.

CPP 12.8 Mon 16:30 Poster C

**Excited states in hole-transporting polymers for phosphorescent OLEDs**— ●BIANCA HÖFER<sup>1</sup>, MANUEL THESEN<sup>2</sup>, SILVIA JANIETZ<sup>2</sup>, HARTMUT KRÜGER<sup>2</sup>, and ANNA KÖHLER<sup>1</sup> — <sup>1</sup>University of Bayreuth, Experimental Physics II, Bayreuth, Germany — <sup>2</sup>Fraunhofer Institute of Applied Polymer Research, Potsdam, Germany

Organic light-emitting diodes (OLEDs) have by now demonstrated efficiencies that enable applications not only for display functions but also for lighting purposes. Current efficient OLEDs are typically fabricated using host-guest-systems. The investigation of excited state formation can help to find ways to suppress efficiency lowering effects like intermolecular excited states. Understanding of the underlying inter- and intra-molecular processes that lead to the formation of excited states can help to optimise host materials. Here we present a comparative spectroscopic study of six hole-transporting materials. These materials consist of a polystyrene backbone with triphenylamine derivatives as pendent side chains. Absorption and photoluminescence measurements as well as time resolved spectroscopy were used to assign emission from singlet, triplet and intermolecular states and determine the transition rates between these states. Furthermore, we discuss the relation between chemical structure and formation of intermolecular states.

CPP 12.9 Mon 16:30 Poster C

**Exciton transfer in light-harvesting systems** — ●JÖRG LIEBERS,

CARSTEN OLBRICH, and ULRICH KLEINEKATHÖFER — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

The exciton dynamics in the light-harvesting 2 system (LH2) of purple bacterium are studied with a quantum-classical approach that combines molecular dynamics simulations (MD) with quantum chemistry calculations and quantum dynamical simulations. To obtain the thermal fluctuations of the nuclear positions of the LH2 ring embedded in a membrane, all-atom classical MD simulations were performed. The results of these simulations serve as an input for quantum chemical calculations to determine the energies of the  $Q_y$  excited states of the single Bacteriochlorophyll (BChl) molecules. From the results of these calculations we construct a time-dependent Hamiltonian of the LH2 exciton system and the spectral density which describes the interaction of the BChl system and the environment. The exciton dynamics are simulated using two different formalisms. A density matrix approach using the spectral density [1,2] and wave packet dynamics based on the time-dependent Hamiltonian. To compare our approach to experimental results, optical spectra of the LH2 complex are calculated.

[1] U. Kleinekathöfer, J. Chem. Phys. **121**, 2505 (2004).[2] U. Kleinekathöfer, I. Barvik, P. Herman, I. Kondov and M. Schreiber, J. Phys. Chem. B **107**, 14 094-14 102 (2003).

CPP 12.10 Mon 16:30 Poster C

**Transport through a wire with fluctuating site energies** —

●BOGDAN POPESCU, LISA MOEVIUS, and ULRICH KLEINEKATHÖFER — Jacobs University Bremen, Campus Ring 1, 28759, Bremen, Germany

In the present work, the electron transport through a molecule, modeled as a linear chain of tight-binding sites and weakly coupled to external leads, is investigated using a reduced density matrix formalism. A quantum master equation is used in the framework of second-order perturbation theory to describe the dynamics of electrons passing through the molecular wire [1]. The advantage of our method is the accurate treatment of time-dependent effects such as external laser pulses [2]. Our method is applied to compute the electrical current through a molecule, such as DNA, where the site energies and the nearest-neighbor couplings are time dependent because of solvent effects. Moreover, the results are compared to coherent transport calculations on the basis of Landauer theory.

[1] S. Welack, M. Schreiber and U. Kleinekathöfer, The influence of ultra-fast laser pulses on electron transfer in molecular wires studied by a non-Markovian density matrix approach, J. Chem. Phys. **124**, 044 712-1-9 (2006).[2] G.-Q. Li, S. Welack, M. Schreiber and U. Kleinekathöfer, Tailoring current flow patterns through molecular wires using shaped optical pulses, Phys. Rev. B **77**, 075 321-1-5 (2008).