CPP 40: POSTERS Electronic and Optical Properties

Time: Thursday 17:00–19:30

Optimization of the Photochromic Response of Photo-Addressable Polymers with Azobenzene-Containing Molecular Glasses — \bullet HUBERT AUDORFF¹, LOTHAR KADOR¹, ROLAND WALKER², and HANS-WERNER SCHMIDT² — ¹University of Bayreuth, Institute of Physics and BIMF, D-95440 Bayreuth, Germany — ²University of Bayreuth, Macromolecular Chemistry I and BIMF, D-95440 Bayreuth, Germany

A new series of photochromic molecular glasses has been synthesized and investigated as blending materials for improving the photochromic response of photoaddressable diblock copolymers. We performed a detailed study of the optical properties of the new materials in correlation with their structural properties. Various end groups as well as different core compounds are employed to achieve a combination of high thermal stability, good sensitivity, and high refractive index modulation. To obtain a better understanding of the photochromic response behavior of our materials, we performed the holographic experiments under a variety of conditions, e.g. at elevated temperatures and on blends with polystyrene and an azobenzene-containing homopolymer. In a blend of the molecular glass with polystyrene, 20 plane-wave holograms were recorded at the same spot by angular multiplexing. By doping the photochromic molecular glass into photoaddressable diblock copolymers, we accomplished an increase of the comparably low sensitivity of the latter, which is the biggest drawback of polymer materials. To increase the sensitivity even further, the holographic grating can be inscribed at elevated temperatures.

CPP 40.2 Thu 17:00 P3

High resolution single molecule spectroscopy of dye in different environments. — •STEFAN KRAUSE, JÖRG SCHUSTER, and CHRISTIAN VON BORCZYSKOWSKI — Center of nanostructured materials and analytics, TU Chemnitz, 09107 Chemnitz

The use of functionalized dyes for fluorescence labelling has introduced a lot of new branches especially in the fields of physics, medicine and biology. Thus, investigating orientation and conformation of bound functionalized molecules is the key to various new applications. According to recent publications on perylene-dyes their spectral properties are very sensitive to conformations of the dye backbones. Hence more detailed single molecule investigations by high resolution fluorescence spectroscopy at low temperature with narrow band dye lasers are a first step to understand the physical processes within these complex systems. Especially the influence of different environments given by the binding of the label on the target surface or the interaction with quantum dots on spectral positions and line widths are of interest [1]. Here we present first results we obtained on surface bound perylene using a home built low temperature single molecule microscopy and spectroscopy setup.

[1] E.I. Zenkevich, C. von Borczyskowski, J. Lum., 122, 784, 2007

CPP 40.3 Thu 17:00 P3

Lowest ionization energies of transition metal ions in aqueous solutions investigated by photoelectron spectroscopy — •ROBERT SEIDEL¹, MANFRED FAUBEL², WOLFGANG EBERHARDT¹, and BERND WINTER¹ — ¹Helmholtz Zentrum Berlin/BESSY II, Albert-Einstein-Strasse 15, 12489 Berlin, Germany — ²Max-Planck-Institut für Dynamik und Selbstorganisation, Bunsenstrasse 10, 37077 Göttingen, Germany

Hydration structure and electron energies of solvated ions are crucial for their reactivity in aqueous solutions. Here we report photoemission spectra from aqueous transition metal ions, which serve as homogeneous and heterogeneous catalysts. From the spectra the experimental vertical ionization energies of Ag^+ , Fe^{2+} , Fe^{3+} , and Cu^{2+} in water are obtained for the first time. The experiments were performed at the soft X-ray U41 PGM undulator beamline at BESSY II. A specially designed liquid microjet, providing a free liquid surface in vacuum, enables the detection of photoelectrons from the highly volatile solutions. A number of inorganic salt solutions are systematically investigated. One focus is on correlating measured electron binding energies, obtained for different counter ions and concentrations, with solvation shell structural details. Experimental binding energies are compared with theoretical calculations.

Location: P3

CPP 40.4 Thu 17:00 P3

Increasing conjugated polymer film conductivity by charge transfer complexes — •FATEMEH GHANI¹, JÖRN-OLIVER VOGEL¹, GEORG HEIMEL¹, JÜRGEN P. RABE¹, NORBERT KOCH¹, SEYFULLAH YILMAZ², SYBILLE ALLARD², and ULLRICH SCHERF² — ¹Institut f. Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — ²Fachgebiet Makromolekulare Chemie, Fachbereich C - Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, 42119 Wuppertal, Germany

Charge transfer complexes formed by mixing the molecular acceptor tetrafluoro-tetracyanoquinodimethane (F4TCNQ) with different donor materials (based on oligothiophene/quinoxaline copolymers) in thin films were investigated. Infrared absorption spectroscopy was used to quantify the donor-acceptor charge transfer as function of acceptor concentration. Furthermore, current/voltage curves of such thin films were measured, and a pronounced increase of the conductivity was found for increasing acceptor concentration (up to three orders of magnitude). However, the dependence of the conductivity on acceptor concentration was sub-linear, implying that the charge carrier mobility was reduced upon charge transfer complex formation.

CPP 40.5 Thu 17:00 P3 Influence of electrochemical cell construction at impedance spectroscopy measurements — MATTHIAS HAASE, •PATRYK HALLEK, and VOLKER BUCK — University Duisburg-Essen, Department of Technical Physics, Germany

The degradation of materials which follow-up to corrosion is one of the most important problems. Particular identification of processes, which take place at the surface of materials, helps to improve the properties of anticorrosion coatings. One of the best method to study corrosions processes is the Electrochemical Impedance Spectroscopy (EIS). This method gives the possibility to recognize very well the change of the surface properties through corrosion products, but a wrong layout of the electrochemical cell can take strong influence at the results.

This work describes the influence of the construction of an electrochemical cell at the measured impedance spectra. For the measurements a three electrode system was established by using either a glass and a plastic chamber. A platinum foil was used as a counter electrode. As a reference electrode and pseudo-reference electrode we took a silver chloride electrode or a platinum rod, respectively.

The measured spectra show a strong interaction between the three electrodes. The impedance plots contain several artifacts in form of capacitive and inductive arcs. This arcs are not correlated with the corrosion process, but they influence on the correct interpretation of the results and choice of an equivalent electric network. The experiments shows that this effects can be minimized by the optimization of the electrochemical cell construction.

CPP 40.6 Thu 17:00 P3 Chemical etching of the tips for SNOM-Raman Microscope

— •DARIA KOVALENKO, MARTIN KÜTTNER, and JÖRG OPITZ — Fraunhofer Institut IZFP Dresden Deutschland

In this paper we will present our results concerning tip preparation for an instrument combining the SNOM and the Raman techniques of probe analysis. Like in SNOM and other kinds of optical microscopy, the resolution depends on the shape and properties of the tip. There are different ways of the tip preparation. In our case the etching is used. The tip etching was held in a two-layer solution: the lower layer consisted of 40 % hydrofluoric acid (HF), the upper layer was an organic solvent, such as toluol or cyclohexane. The time and the temperature of etching were varied. The dependences between the tip shape and the parameters of the etching were carried out. The optimal time of etching the fiber ranges from 90 to 120 min. The temperature of the etching depends strongly on the physical properties of the solvent. Typically a temperature of abut 15-25 oC is used. For higher temperatures of the etching solution a faster etching is observed. The density of the solvent influences the lubricity of the surface and also the tip angle. The best results (tip angle equals 900) are able to obtain in the solvent with density of about 0.90 * 1.05 g/cm3.

 $\label{eq:CPP} \begin{array}{c} {\rm CPP} \ 40.7 \quad {\rm Thu} \ 17:00 \quad {\rm P3} \\ {\rm A \ tunable \ subwavelength \ microresonator \ design \ for \ inves-} \end{array}$

tigation of single quantum emitters — •RAPHAEL GUTBROD¹, ALEXEY CHIZHIK¹, ANNA CHIZHIK¹, DMITRY KHOPTYAR², and ALFRED J. MEIXNER¹ — ¹Institute of Physical and Theoretical Chemistry, University of Tübingen, Auf der Morgenstelle 8, 72076 Tübingen, Germany — ²Department of Physics, Lund University, Box 118, S-221 00 Lund, Sweden

Optical microresonators are structures which confine light to a small volume in the range of one wavelength. Our system is based on a Fabry-Perot $\lambda/2$ -microresonator and can be reversibly tuned across the whole visible spectral range. This has great potential for intra-cavity studies and can be used to modify the optical properties of a definite single quantum emitter. We present here experimental and theoretical results on modification of the fluorescence emission spectrum as well as the spontaneous emission rate of a single molecule embedded in the microresonator. Additionally, a single fluorescent bead is used to probe the change of the intra-cavity excitation field during resonator tuning. We use radially and azimuthally polarized doughnut mode laser beams for excitation and compare the result with calculated patterns. These beams show an excitation pattern which has distinct features in different parts of the microresonator. This allows us to determine the position of the fluorescent bead with an accuracy of a few nanometres. Furthermore, we also use these beams to determine the orientation of single molecules in the microresonator.

 $CPP \ 40.8 \quad Thu \ 17:00 \quad P3$

Dynamical screening of an endohedral atom — •STEPHANIE Lo¹, ANDREI KOROL^{1,2}, and ANDREY SOLOV'YOV¹ — ¹FIAS, JW Goethe University, Frankfurt am Main, Germany — ²Department of Physics, St. Petersburg State Maritime Technical University, St. Petersburg, Russia

The present work is a generalisation of the dynamical screening factor presented in [1] to consider an atom located at an arbitrary position within the fullerene. A more elaborated investigation into the case where the atom is located at the centre is performed and compared with quantum mechanical calculations for dynamical screening factor of Ar@C₆₀ [2] and Mg@C₆₀ [3]. The π and σ plasmons of the fullerene are accounted for in a modified screening factor to improve correspondence with the quantum calculations. The spatial dependence of the screening factor was explored with Ar@C₆₀ and Ar@C₂₄₀ and found to depend significantly on the radial distance of the atom from the centre of the fullerene. A spatial averaging of the screening factor is presented. The dynamical screening of an endohedral molecule is also being considered.

References

[1] Lo S, Korol A V and Solov'yov A V 2007 J. Phys. B: At. Mol. Opt. Phys. $\mathbf{40}$ 3973–81

[2] Madjet M E, Chakraborty H S and Manson S T 2007 Phys. Rev. Lett. ${\bf 99}$ 243003

[3] Chakraborty H S, Madjet M E, Rost J-M and Manson S T 2008 Phys. Rev. A 78 013201

CPP 40.9 Thu 17:00 P3

About the molecular weight and temperature dependence of the microstructure of regioregular poly(3-hexylthiophene) — •ZHIYONG WU¹, ALBRECHT PETZOLD¹, THOMAS THURN-ALBRECHT¹, RUTH LOHWASSER², MICHAEL SOMMER², and MUKUNDAN THELAKKAT² — ¹Institut für Physik, Martin-Luther-Universität Halle-Wittenberg — ²Makromolekulare Chemie I, Universität Bayreuth

We report about structural investigations of a series of regionegular poly(3-hexylthiophene) (P3HT) with different, well defined molecular weight using a combination of x-ray scattering techniques (WAXS, SAXS) and calorimetry (DSC). The semicrystalline structure of P3HT shows a complex temperature dependence. It undergoes a solid-to-solid phase transition at around 60°C and melting occurs in two steps with an intermediate layered structure with smectic symmetry. Wide angle x-ray diffraction (WAXD) experiments give evidence for an orthorhombic crystal unit cell consistent with previous reports in the literature. We propose a structure at room temperature with polyethylene-like packing of the side chains tilted with respect to the main chains and without interdigitation. At the phase transition side chain melting occurs and the side chains acquire a disordered state. The corresponding ordering process during cooling is kinetically hindered for higher molecular weight. DSC measurements show, that the melting temperature as well as the enthalpy of melting strongly increase with increasing molecular weight, indicating an increase both of the thickness of the crystallites and of the crystallinity. This result is confirmed by direct structural analysis using small angle x-ray scattering.

CPP 40.10 Thu 17:00 P3 Femtosecond Transient Absorption of a Polyfluorene Copolymer at High Hydrostatic Pressure — •SEBASTIAN ALBERT-SEIFRIED — Cavendish Laboratory, University of Cambridge, J. J. Thompson Avenue, Cambridge CB3 0HE, United Kingdom

Organic light emitting diodes (OLED) are currently considered lowcost alternatives to established illumination and display technologies. However, the two main problems faced by OLED technologies are short device lifetime and low energy efficiency. To address these shortfalls, it is critical to understand the photophysics of conjugated polymers in the solid state, which are often more complex than in their inorganic counterparts due to the ill-defined interaction of neighbouring molecules.

Applying high pressure is a clean reversible way to increase the interchain interactions and thus study their effects on conjugated polymers. For this purpose, a technique was developed to study ultrafast dynamics of excitation under hydrostatic pressure up to 90 kbar by transient absorption over the whole visible spectrum. In thin films of poly(9,9di-n-octylfluorene- alt-benzothiadiazole) (F8BT) at high hydrostatic pressure, a strong dynamic relaxation of the stimulated emission by around 200meV was found after excitation. Further, a sharp decline of stimulated emission and photoluminescence with increasing pressure was measured. The pressure dependent spectrscopy is interpreted in terms of interchain and intrachain effects on radiative and nonradiative processes.

CPP 40.11 Thu 17:00 P3

Terahertz Time Domain Spectroscopy of PEDOT:PSS conducting polymer for photovoltaic devices — •MONIKA WEBER¹, KONRAD VON VOLKMANN¹, TOBIAS KAMPFRATH³, MARTIN SCHEUCH¹, INGO SALZMANN², CHRISTIAN FRISCHKORN¹, NORBERT KOCH², and MARTIN WOLF¹ — ¹Institute of Experimental Physics, Freie Universität Berlin — ²Physics Institute, Humboldt-University Berlin — ³FOM Institute for Atomic and Molecular Physics [AMOLF], Amsterdam

The number of polymer based devices grows very fast. Almost all of them, like organic field effect transistors, electro luminescent panels, LEDs or photovoltaic cells, use conducting layers. One of widely used intrinsic conducting polymers is poly-(3,4-ethylenedioxythiophene) complex with sulfonic acid also known as PEDOT:PSS. Understanding of charge transfer in PEDOT:PSS is still lacking.

Here, we present first measurements of PEDOT:PSS thin films measured with terahertz time domain spectroscopy in a frequency range between 8 THz and 32 THz. THz TD spectroscopy allows us to determine the complex dielectric function and conductivity. Temperature-dependent measurements give information about charge transfer.

CPP 40.12 Thu 17:00 P3

Charge Trapping and Color Stability in a White-Emitting Copolymer — •SEBASTIAN BANGE and DIETER NEHER — Universität Potsdam, Institut für Physik und Astronomie, Karl-Liebknecht-Str. 24–25, 14476 Potsdam-Golm, Germany

Organic white light-emitting devices are of considerable interest as a technology capable of providing low-cost, potentially highly efficient lighting. Precise control over the emission color is especially difficult for polymeric devices, where several chromophores compete for excitations within a single active layer.

We investigate the role of charge trapping for the emission color of polymeric light-emitting devices comprising a copolymer based on polyspirofluorene with additional hole transporting units and blue, green and red singlet emitting moieties. Strong influence of drive parameters on the emission spectrum are observed and explained by an analytic model accounting for charge trapping on the red dye. Contrary to purely kinetic arguments[1], this model allows to understand the effects of electrode modifications and provides insight into interface conditioning effects[2] during operation.

[1] Gather et al., Advanced Materials 19, 4460 (2007)

[2] Bange et al., Journal of Applied Physics 104, 104506 (2008)

CPP 40.13 Thu 17:00 P3

Hydrogen storage in charge compensated organic molecular crystals — •MINA YOON^{1,2} and MATTHIAS SCHEFFLER¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — ²Oak Ridge National Laboratory, USA

We propose charge compensated organic molecular crystals as a

promising class of materials for hydrogen storage. Using quantum mechanical first-principles calculations based on numerical atom-centered orbitals as all-electron basis functions [1] we study the basic structural properties of molecular crystals consisting of parallel sheets of cations and anions (such as DMPH and TCNQ) stacked alternatingly. The long range dispersion interactions between the cations and anions, which are important for the stability of the crystals, were studied and compared using various DFT xc functionals, semi-empirical approach [2], and Møller-Plesset perturbation theory. The molecular configuration causes accumulation of electrons at acceptors and depletion at donors, which results in finite dipolar fields. Our study indicates that these fields make it possible to use charge compensated organic molecular crystals for hydrogen storage.

[1] V. Blum *et al.*, FHI ab initio molecular simulations (FHI-aims) project. [2] A. Tkatchenko and M. Scheffler, to be published.

CPP 40.14 Thu 17:00 P3

Surface and structure analysis of thin MEH-PPV:PVK polymer blend films — •ROBERT MEIER¹, MATTHIAS A. RUDERER¹, GUNAR KAUNE¹, ALEXANDER DIETHERT¹, STEPHAN V. ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department LS E13, James-Franck-Straße 1, 85747 Garching — ²HASYLAB at DESY, Notkestraße 85, 22603 Hamburg

The surface and inner structure of novel thin blend films of photoactive conjugated polymers are investigated. Conjugated polymers in thin films become of great interest for versatile applications such as organic thin film transistors, light emitting diodes or photovolatics. We focus on blend films based on MEH-PPV (poly[2methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene]) and PVK (poly N-vinylcarbazole) which are prepared with spin coating. It has been shown that, due its charge transfer properties, MEH-PPV is a very promising candidate for applications [1]. The thin films show phase separation at the microscale, which turned out to be very well tuneable via the polymer concentrations in their solution used for preparation. The film surface is characterized by using atomic force microscopy and imaging ellipsometry and the inner film structure is analysed with GIUSAXS and GISANS measurements. The investigation is complemented by probing the conducting properties of the polymer blend films and their light absorbing abilities using UV-Vis spectroscopy.

[1] R. Meier et. al., Physical Review B 77, 195314 (2008)

CPP 40.15 Thu 17:00 P3

The role of exciplexes in phoshorescent host-guest systems — •BIANCA HÖFER¹, MANUEL THESEN², HARTMUT KRÜGER², SILVIA JANIETZ², and ANNA KÖHLER¹ — ¹Department of Physics, University of Bayreuth, 95440 Bayreuth, Germany — ²Fraunhofer Institute of Applied Polymer Research, 14476 Potsdam, Germany

Efficient organic white light emitting diodes (OLEDs) can be produced using several organometallic phosphorescent dyes embedded in an organic matrix. We recently demonstrated that steric shielding can be employed to avoid cascading energy transfer from blue to red emitting dyes in a blend of Ir-complexes using polymeric oxadiazole- and triphenylamine-derivatives as electron and hole transporting materials.* Here we investigate the dynamics of energy transfer between the emissive dyes and the host materials. We address the issue how nonemissive exciplexes in the host materials may control the efficiency of the white OLEDs.

CPP 40.16 Thu 17:00 P3

Intermolecular coupling in low polydispersity poly(3-hexylthiophene)s — •CHRISTINA HACKE¹, BIANCA HÖFER¹, RUTH LOHWASSER², MUKUNDAN THELAKKAT², and ANNA KÖHLER¹ — ¹Department of Physics, University of Bayreuth, 95440 Bayreuth, Germany — ²Department of Chemistry, University of Bayreuth, 95440 Bayreuth, Germany

The optical and electronic properties of regioregular poly(3hexylthiophene) (P3HT) are of great interest for many applications in the field of organic semiconducting materials such as solar cells and field-effect transistors (OFETs). Recent research has highlighted the strong dependence of charge carrier mobility in the conformation of the P3HT backbone and the resulting intermolecular interactions. The formation of weakly interacting aggregates in P3HT depends strongly on molecular weight. Here we use P3HT with a very low polydispersity to study the molecular weight dependence in the formation of such aggregates. To assess the intermolecular interaction and the resulting morphology of the film, we use absorption measurements in solutions and films in combination with atomic force microscopy.

CPP 40.17 Thu 17:00 P3

The oligomer length dependence of triplet excition diffusion in polyfluorenes — •SEBASTIAN T. HOFFMANN¹, LEKSHMI SUDHA DEVI¹, IRENE BAUER¹, ESTHER SCHELER², PETER STROHRIEGL², and ANNA KÖHLER¹ — ¹Department of Physics, University of Bayreuth, 95440 Bayreuth, Germany — ²Department of Chemistry, University of Bayreuth, 95440 Bayreuth, Germany

Triplet excitons play an important role in organic light emitting diodes and solar cells. However, very little is known about the mechanism by which the triplet excitons move and the microscopic parameters which govern triplet (Dexter) energy transfer in conjugated polymers. For a heavy metal containing conjugated polymer and its associated monomer, we have recently shown that triplet diffusion occurs by quantum mechanical tunneling at low temperatures and by thermally activated hopping above a transition temperature. [1,2]. In the present study, we extend our investigation to a PF2/6 polymer, trimer and dimer. We find that for the polyfluorene compounds, triplet diffusion can be described by the same model. As theoretically predicted2, the activation energy in the hopping regime and the transition temperature between the hopping and the tunnelling regime decreases with oligomer length. We discuss the influence of disorder on the transport process.

References [1] L. S. Devi, M. K. Al-Suti, C. Dosche, M. S. Khan, R. H. Friend, and A. Kohler, Physical Review B 78 (2008). [2] I. I. Fishchuk, A. Kadashchuk, L. S. Devi, P. Here-mans, H. Bassler, and A. Kohler, Physical Review B 78 (2008).

CPP 40.18 Thu 17:00 P3 **A model for triplet exciton diffusion in poly(para-phenylene) derivatives** — •ANNA KÖHLER¹, SEBASTIAN HOFFMAN¹, LEKSHMI SUDHA DEVI¹, MICHAEL FORSTER², JAN-MORITZ KOENEN², and ULL-RICH SCHERF² — ¹Department of Physics, University of Bayreuth, 95440 Bayreuth, Germany — ²Department of Chemistry, Bergische Universität Wuppertal, Wuppertal, 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 have recently shown that, for an organometallic polymer with low energetic disorder, triplet diffusion can be described in the framework of the Holstein small polaron model.(1,2) It predicts a tunnelling process at low temperatures followed by a thermally activated hopping process above a transition temperature. Using phosphorescence measurements, we have here investigated the dynamics of triplet diffusion in the polyfluorene PF2/6 and the ladder-type poly(para-phenylene) MeLPPP. We find this model is suited to describe the dynamics of triplet diffusion in these organic polymers and oligomers. The dominant parameter that controls the triplet transfer rate is the relative size of polaronic effects to energetic disorder. Experimentally, we show that the triplet diffusion rate increases with decreasing geometric relaxation energy and disorder.

(1) L. Sudha Devi et al, PRB 78, 45210, 2008. (2) I. I. Fishchuk et al, PRB
78, 45211 2008.

CPP 40.19 Thu 17:00 P3

Electroactive Polymers for Flexible and Conformable Touchpads and Keyboards — •GERDA BUCHBERGER, REINHARD SCHWÖDIAUER, NIKITA ARNOLD, and SIEGFRIED BAUER — Johannes Kepler Universität, Linz, Österreich

Cellular polypropylene ferroelectrets are flexible, lightweight and piezoelectric transducer materials, which are used in a wide range of sensing applications. We fabricated and characterized a ferroelectret touchpad of 10x10 cm². It consists of a ferroelectret film that is placed between two large area electrodes. Electrical ports are fixed to the corners of the device. If a force is applied, transient voltage signals can be measured due to the piezoelectric effect. The voltage amplitudes depend on the touch position. In addition to the touchpad we fabricated keyboards using a binary coding technique profiting from the polarization states of the ferroelectret. Functional layers with a polarization pattern are covered by large area electrodes and stacked afterwards. The keys are encoded by the sequence of the polarization states. If a force is applied to a key, the corresponding transient voltage signals are measured at the edges of the device for every layer. As the polarization pattern and therefore the signal sequence is characteristic for every key it can be determined unambiguously. As we use large area electrodes combined with contacts only at the edges, sensor matrices are avoided. The concepts can be further extended to flexible transparent devices using polyvinylidene fluoride and transparent electrodes. The devices may

be used for rollable touchpads and keyboards, for consumer goods as intelligent price tags and for whole body tactile sensors.