

## CPP 10: POSTERS New Materials, Organic Semiconductors

Time: Monday 16:45–19:00

Location: Poster A

CPP 10.1 Mon 16:45 Poster A

**Optical properties of Biaxial Nematogens** — ●DAVID POLSTER<sup>1</sup>, CHRISTIANE KÖHN<sup>2</sup>, JENS SELTMANN<sup>2</sup>, MATTHIAS LEHMANN<sup>2</sup>, HARALD GRAAF<sup>1</sup>, JÖRG SCHUSTER<sup>1</sup>, and CHRISTIAN VON BORCZYKOWSKI<sup>1</sup> — <sup>1</sup>Center of Nanostructured Materials and Analytics, TU Chemnitz, 09107 Chemnitz, Germany — <sup>2</sup>Juniorprofessur Nichtklassische Synthesemethoden, TU Chemnitz, 09107 Chemnitz, Germany

Typical liquid crystalline molecules (nematogens) are characterized by a linear shape with one permanent dipole and are known to form a nematic phase. In biaxial nematogens (V-shaped molecules) instead two perpendicular dipoles can be found. For such mesogens the tendency to form the so illusive biaxial nematic phase is proposed for which up to 100fold faster switching times are expected.

We will present here a new class of unsymmetric substituted V-shape molecules. These mesogens consists of a bent core which defines the dihedral angle of the V-shaped molecule and two rigid arms with cyano substituted terminal aromatic units. They are characterized by two different dipole moments along the short and the long molecular axis. The thermotropic behavior of these new materials has been investigated and its nematic phase was characterized. The orientation of the nematogens in a typical liquid crystal cell will be shown and the influence of an applied electric field will be discussed. An alignment along the short axis of the molecule under electric field plays the major role for low voltages.

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**Switchable Fluorescence Cell** — ●FRANK FRIEDRISZIK, HARALD GRAAF, JÖRG SCHUSTER, and CHRISTIAN VON BORCZYKOWSKI — Center of Nanostructured Materials and Analytics, TU Chemnitz, 09107 Chemnitz, Germany

Calamitic liquid crystalline materials are well known and used in a wide spread of display applications. One of the most common material is the 4-pentyl-4-cyanobiphenyl (5CB) which is in the nematic phase at room temperature. Rubbed polyimide films can be used for an orientation of these calamitic liquid crystals in a liquid crystal cell where the molecules are aligned parallel to the substrate and with its axis along the rubbing direction. Due to the permanent dipole moment of the LC molecule an applied electric field perpendicular to the substrate surface will switch the orientation of the molecules parallel to the electric field.

Here we present recent results on the alignment of a rod like organic dye molecule doped into the liquid crystal and which orients within the liquid crystal parallel to the 5CB molecules. Thus, in the liquid crystal cell the organic molecules are oriented parallel to the substrate surface and its orientation will be switched together with the liquid crystal in an electric field. As the transition dipole of the dye molecule is oriented along the axis of the molecule its luminescence is also switched by the electric fields. Thus we are able to demonstrate a prototype of a switchable fluorescence cell. Besides potential display applications, such a dye which aligns with the liquid crystal is also a perfect probe of local liquid crystal structure.

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**Chemical modification and radiation induced degradation of the photoresist SU-8** — ●ANGELA KEPPLER<sup>1</sup>, MARCEL HIMMERLICH<sup>1</sup>, CHRISTOPH KREMIN<sup>1</sup>, JENS T. SCHUMACHER<sup>2</sup>, ANDREAS GRODRIAN<sup>2</sup>, JUERGEN A. SCHAEFER<sup>1</sup>, JOSEF METZE<sup>2</sup>, MARTIN HOFFMANN<sup>1</sup>, and STEFAN KRISCHOK<sup>1</sup> — <sup>1</sup>Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany — <sup>2</sup>Institut für Bioprozess- und Analysenmesstechnik e.V., Rosenhof, 37308 Heilbad Heiligenstadt, Germany

An increasing interest in using the epoxy-based photoresist SU-8 for producing bio-MEMS or microfluidic devices is noticeable. In biological applications, sterilisation processes using chemical treatments or UV radiation are common practice and the analysis of their interaction with SU-8 is of great interest. Employing X-ray photoelectron spectroscopy and contact angle measurements, we have investigated the changes in the surface chemical composition upon IR, UV and X-ray irradiation as well as the impact of contact with chemicals. The treatment of SU-8 with H<sub>2</sub>SO<sub>4</sub> results in oxidation (formation of C=O bonds) while at NaOH treated surfaces, a reduction of ether bonds is found. Radiation induced changes and degradation of the polymer in-

duced by X-ray, UV and IR irradiation were characterised. In contrast to X-ray and IR radiation where no modification was found, UV photons preferentially attack the ether bonds in SU-8, resulting in a strong degradation of the material. The chemical changes are correlated to differences in the contact angle of the material as well as its optical properties.

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**A co-axial dielectric elastomer actuator** — ●HRISTYAN STOYANOV, GUGGI KOFOD, and REIMUND GERHARD — Applied Condensed-Matter Physics, University of Potsdam, Am Neuen Palais 10, D-14469 Potsdam, Germany

Dielectric elastomer actuators based on Maxwell-stress induced deformation, are considered for many potential applications where high actuation strain and high energy density are required. They usually rely on a planar actuator configuration, however, a string-like actuator would be less bulky, and more versatile for several applications. A co-axial dielectric elastomer actuator was developed and evaluated. The proposed geometry is fabricated through alternating dip-coating steps with thin insulating and conductive elastomer layers. Actuators with single and multiple active layers have been successfully demonstrated. The actuation strain and force generated by the actuators were determined at different levels of pre-strain. Voltage-dependent actuation strain measurements were obtained. The experimental results were compared to a straightforward electromechanical model for cylindrical elastomer actuators.

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**Nano/micro-structure formation driven by local protonation of polymer thin films via dip-pen nanolithography** — ●CARSTEN MÄDLER<sup>1,2</sup>, SAILAJA CHADA<sup>2</sup>, ANDRES LA ROSA<sup>2</sup>, and MINGDI YAN<sup>2</sup> — <sup>1</sup>Center of Nanostructured Materials and Analytics, TU Chemnitz, 09107 Chemnitz, Germany — <sup>2</sup>Portland State University, PO Box 751, Portland OR 97207, US

While dip-pen nanolithography uses a sharp tip to anchor molecules on the substrate to form nanostructures, an alternative approach is presented here to exploit the responsiveness of the substrate. Acidic phosphate buffer molecules are delivered into ultraviolet-crosslinked films to swell the polymer material by a protonation-based mechanism. The experiment aims to provide the first demonstration of stimulating the mechanical response of polymer materials by confining protonation reaction locally and in a controlled manner. A series of experiments suggests that the structures are indeed due to swelling of the polymer. The process was studied at different dwell times and contact forces. A dependence of the structure height on the contact force was found, which is rather unusual for DPN processes.

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**Charge transfer between covalently bound oligothiophenes and fullerene** — ●WICHARD J D BEENKEN — Technische Universität Ilmenau, FG Theoretische Physik I, Weimarer Str. 25, 98693 Ilmenau

Understanding the charge transfer between conjugated polymers, esp. poly-thiophenes, and fullerenes or their derivatives is of high interest, since this is the key process for polymer-based organic solar cells. Nevertheless, there exist only very few theoretical studies about this system. The main problem is the undefined conformation between the two constituents. Using quantum-chemical methods, esp. TD-DFT, we calculated several oligo-thiophenes of various lengths, which were covalently bound to the fullerene C<sub>60</sub>. We identified several charge transfer states by plotting the respective charge-difference densities. Thereby it turns out that the kind of bridge between thiophene and C<sub>60</sub> is crucial for the charge transfer energetics. We will show how one may try to eliminate this effect.

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**Supermolecular structure and charge carriers mobilities of perylene diimides** — ●VALENTINA MARCON<sup>1</sup>, JAMES KIRKPATRICK<sup>1,2</sup>, WOJTEK PISULA<sup>1</sup>, and DENIS ANDRIENKO<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für Polymerforschung, Mainz, Germany — <sup>2</sup>Department of Physics, Imperial College London, London, United Kingdom

Perylene diimides form columnar phases, where the molecules stack on

top of each other and the columns arrange in a regular lattice. The self-organization into well-ordered columns results in the one-dimensional charge transport along the stack of the aromatic cores of the molecules. Most of the discotic molecules which organize in columns are p-type semiconductors, while the class of rylene diimide molecules, to which perylene belongs, forms n-type organic semiconductors.

Using atomistic molecular dynamics (MD) simulations we study the columnar phases of perylene diimides and establish correlations between the molecular structure, packing, and dynamical properties of these materials.

By using a scheme which combines electronic structure calculations, MD and kinetic Monte Carlo simulations, a correlation is then established between the molecular structure and charge mobility of perylenes columnar mesophases.

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**Atomistic force field and electronic properties of carbazole: melt and macrocycle** — ●THORSTEN VEHOFF<sup>1</sup>, JAMES KIRKPATRICK<sup>2</sup>, KURT KREMER<sup>1</sup>, and DENIS ANDRIENKO<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany — <sup>2</sup>Department of Physics, Imperial College London, Prince Consort Road, London SW7 2B W, United Kingdom

Processable polymers with a conjugated backbone, e.g. carbazole, are interesting for use as hole conducting materials. Hole transport characteristics strongly depend on the local arrangement of molecules; for this reason, to obtain an efficient device, it is necessary to control the morphology of the material: very often, small changes of the structure (e.g. longer alkane side chains) or processing conditions (annealing regime, choice of solvents) result in a significant change of the morphology and, hence, charge carrier mobility.

In this contribution, we study the columnar mesophase of a carbazole macrocycle. First an atomistic force field is developed for carbazole furnished with alkyne side chains as well as carbazole dimers and then tested on a melt of carbazole oligomers by evaluating properties such as the density and diffusion coefficient and comparing with experimental results. The mobility of charge carriers along the columns is calculated by first computing charge hopping rates between carbazole monomers and macrocycles according to Marcus theory and then solving the master equation for charge dynamics.

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**Electronic Excitation Transfer in PPV-Mesoporous Silica Matrix** — ●GIL CLAUDIO<sup>1</sup> and ERIC BITTNER<sup>2</sup> — <sup>1</sup>The University of Houston, 4800 Calhoun Road, Houston, Texas 77204, USA. Currently at the Max Planck Institute for Polymer Research, D-55021 Mainz, Germany — <sup>2</sup>The University of Houston, 4800 Calhoun Road, Houston, Texas 77204, USA.

Electronic excitation transfer as described by Förster theory has been shown to occur in various multi-chromophore systems such as conjugated polymers. The direction of energy transfer towards the low energy states is usually random due to the random distribution of chromophores in the system. Schwartz and co-workers synthesized a system with MEH-PPV conducting polymers inserted in the channels of mesoporous silica matrices. In this system, energy transfers from the high-energy randomly oriented chromophores of polymers outside the channels to the low-energy chromophores inside the well-ordered channels. We calculated several configurations of the polymer-silica matrices and the excitation transfer in these systems. These calculations confirm the energy transfer to the targeted sites as hypothesized

in experiment. Lastly, we present criteria that allow efficient energy transfer to specific targeted areas.

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**Optical and electronic properties of oligothiophene dendrimers** — ●THOMAS HARTMANN and PETER REINEKER — Institute of Theoretical Physics, University of Ulm, 89069 Ulm, Germany

Dendrimers, regular star like polymers, are of interest from a fundamental point of view, but also because of various possible applications, such as in light harvesting systems, in solar cells, as carriers for drug delivery or for gene manipulation, or in catalysis, etc. In our investigation of the dendrimers we have focused on optical and energy transport properties of oligothiophene dendrimers with C<sub>2</sub> symmetry. Our calculation of optical and energy transport properties is based on a Frenkel exciton model. This model takes into account the geometry of the dendrimers, local electronic excitation energies, transfer integrals, and the influence of vibrational degrees of freedom via a stochastic description. We have calculated optical absorption line shapes and the time dependence of the energy transport in dependence on the size of the dendrimer. Furthermore the influence of neighboring thiophenes in different branches of the dendrimers is considered.

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**Investigation of phosphorescent blue organic light emitting diodes** — ●CHIEN-SHU CHIU<sup>1,3</sup>, RALF KRAUSE<sup>2,3</sup>, FRYDERYK KOZLOWSKI<sup>3</sup>, ARVID HUNZE<sup>3</sup>, and WOLFGANG KOWALSKY<sup>1</sup> — <sup>1</sup>Department of Electrical Engineering & Information Technology, Technical University of Braunschweig, Germany — <sup>2</sup>Department of Materials Science VI, University of Erlangen-Nuremberg, Germany — <sup>3</sup>Siemens AG, CT MM 1, Günther-Scharowsky-Str. 1, 91058 Erlangen, Germany

Recently, rapid development of phosphorescent materials has significantly improved the efficiency of organic light emitting diodes (OLEDs). By using efficient phosphorescent emitter materials white OLEDs with high power efficiency values could be demonstrated. But especially blue phosphorescent devices, due to stability issues, need to be further investigated and optimized. In this work, blue OLED devices based on the phosphorescent emitter FIrpic were investigated. Single-carrier hole-only as well as electron-only devices were fabricated and characterized to study the impact of charge carriers on device performance.

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**Optimization of Emission Color and Efficiency of Organic Light Emitting Diodes for Lighting Applications** — ●STEFAN SEIDEL<sup>1,2</sup>, RALF KRAUSE<sup>1,2</sup>, FRYDERYK KOZLOWSKI<sup>2</sup>, GÜNTER SCHMID<sup>2</sup>, ARVID HUNZE<sup>2</sup>, and ALBRECHT WINNACKER<sup>1</sup> — <sup>1</sup>Department of Materials Science VI, University of Erlangen-Nuremberg, Germany — <sup>2</sup>Siemens AG, CT MM 1, Günther-Scharowsky-Str. 1, 91058 Erlangen, Germany

In recent years the performance of organic light emitting diodes (OLEDs) has reached a level where OLED lighting presents an interesting application target. Research activities therefore focus amongst other things on the development of high efficient and stable white light emitting devices. We demonstrate how the color coordinates can be adjusted to achieve a warm white emission spectrum, whereas the OLED stack contains phosphorescent red and green dyes combined with a fluorescent blue one. Detailed results are presented with respect to a variation of layer thicknesses and dopant concentrations of the emission layers. Furthermore the influence of various dye molecules and hence different energy level alignments between host and dopants on color and efficiency will be discussed.