

## DS 18: Poster: Towards Molecular Spintronics, Organic Thin Films, Optical Layers, Vibrational Spectroscopy, Tailoring organic interfaces

Time: Tuesday 14:30–19:30

Location: Poster A

DS 18.1 Tue 14:30 Poster A

**Stability and spin coherence of hydrogen atoms trapped in pure silica zeolite** — ●ROLF SIMON SCHOENFELD<sup>1</sup>, WOLFGANG HARNEIT<sup>1</sup>, and CORMA AVELINO<sup>2</sup> — <sup>1</sup>Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany — <sup>2</sup>Instituto de Tecnología Química UPV-CSIC, Universidad Politécnica de Valencia, Avenida de los Naranjos s/n, 46022 Valencia, Spain

We report the first observation of electron paramagnetic resonance (EPR) of hydrogen atoms trapped in pure silica LTA zeolite after gamma irradiation of n-hexane filled samples. Heating experiments revealed stability up to 80 °C in both air containing and evacuated samples. The small isotropic line width and the low deviation of hyperfine coupling constant and g-factor from the free atom values indicate a minimal distortion of the electron wave function. In addition, spin lattice and spin spin relaxation times T1 and T2 were measured by means of FT EPR. Although relaxation by spin diffusion cannot be excluded, a long spin coherence time of more than 12 microseconds was observed at ambient temperature in an evacuated sample.

DS 18.2 Tue 14:30 Poster A

**Observation of spin switching in a chainlike supramolecular Fe (II) complex observed by STM/CITS** — ●M. STOCKER<sup>1</sup>, A. VOLKOV<sup>1</sup>, M.S. ALAM<sup>1</sup>, V. DREMOV<sup>1</sup>, M. RUBEN<sup>2</sup>, and P. MÜLLER<sup>1</sup> — <sup>1</sup>Institut für Physik der Kondensierten Materie, Universität Erlangen-Nürnberg — <sup>2</sup>Institut für Nanotechnologie, FZ Karlsruhe

Using a home-made microscope and custom-build control electronics and software we performed STM/CITS measurements on a chainlike supramolecular Fe (II) complex. The investigated complex shows spin crossover from a low-spin to a high-spin state in a temperature range between 250-350K. We investigated single and multiple polymer strands deposited onto HOPG surfaces. STM topography was able to resolve single monomers. The CITS technique at ambient conditions showed two distinct monomer species, one highly conducting, the other close to insulating. Furthermore we were able to observe spontaneous reversible switching between the two states. The different conductance can be attributed to the different spin states of the Fe (II) metal center. We discuss the results in terms of spin crossover theories.

DS 18.3 Tue 14:30 Poster A

**Magnetization Tunneling and Quantum Transport in Single Molecule Magnets** — ●NIKOLAOS P. KONSTANTINIDIS<sup>1,2</sup>, MAARTEN R. WEGEWIJS<sup>1,2</sup>, CHRISTIAN ROMEIKE<sup>1</sup>, HERBERT SCHOELLER<sup>1</sup>, and WALTER HOFSTETTER<sup>3</sup> — <sup>1</sup>Institut für Festkörper-Forschung - Theorie III, Forschungszentrum Jülich, 52425 Jülich, Germany — <sup>2</sup>Institut für Theoretische Physik A, RWTH Aachen, 52056 Aachen, Germany — <sup>3</sup>Institut für Theoretische Physik, J. W. Goethe-Universität, D-60438 Frankfurt, Germany

The electric current through a single molecule magnet is investigated theoretically as function of an external magnetic field. We present results for the linear transport regime obtained by the numerical renormalization group (NRG) technique [1], as well as non-linear transport properties obtained using quantum kinetic equations. We predict effects related to the coherent magnetization tunneling generated by the magnetic anisotropy. In particular, we show how non-trivial Kondo and spin-tunneling effects allow for a complete determination of the magnetic properties of such a device by transport experiments.

[1] M. R. Wegewijs, C. Romeike, H. Schoeller and W. Hofstetter, *New J. Phys.* 9 344, (2007).

DS 18.4 Tue 14:30 Poster A

**Identifying the single-molecule spin states by vibronic transport effects** — ●FELIX RECKERMANN<sup>1,2</sup>, MAARTEN R. WEGEWIJS<sup>1,2</sup>, and HERBERT SCHOELLER<sup>2</sup> — <sup>1</sup>Institut für Festkörper-Forschung - Theorie 3, Forschungszentrum Jülich, 52425 Jülich, Germany — <sup>2</sup>Institut für Theoretische Physik A, RWTH Aachen, 52056 Aachen, Germany

We show that an electric current through a mixed-valence dimer molecule can detect the spin states of the electronic excitations without external magnetic field. Mixed-valence complexes are molecules in which an excess electron can tunnel between hetero-valent metal

ions. This tunneling mediates both a ferromagnetic double-exchange interaction between the ionic spins as well as a non-adiabatic electron-vibration (so called vibronic) interaction.

One has to account for the coupling of the electron motion to the breathing mode of the two ionic ligand-shells as well as the breakdown of the Born-Oppenheimer approximation. The resulting entanglement of the electronic and vibrational degrees of freedom can be detected by a sharp dependence of the differential conductance on the electro-mechanical parameters. Furthermore, the double-exchange coupling of the ionic spins and the vibrational motion become correlated. In a three terminal device geometry, this allows one to identify the spin states of the molecule using the FC-effect.

DS 18.5 Tue 14:30 Poster A

**On the electronic structure of cobalt phthalocyanine** — ●THOMAS KROLL<sup>1</sup>, VICTOR YU. ARISTOV<sup>1,2</sup>, OLGA V. MOLODSOVA<sup>1</sup>, VICTOR M. ZHILIN<sup>2</sup>, DENIS V. VYALIKH<sup>3</sup>, BERND BÜCHNER<sup>1</sup>, and MARTIN KNUPFER<sup>1</sup> — <sup>1</sup>IFW Dresden, P.O. Box 270016, D-01171 Dresden, Germany — <sup>2</sup>Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow distr., 142432, Russia — <sup>3</sup>Institute of Solid State Physics, TU Dresden, D-01069 Dresden, Germany

Metal phthalocyanines (MPc) are molecular based systems that contain a transition metal ion in its centre. They have long been attractive materials for fundamental aspects as well as technological interest. Furthermore, metal phthalocyanine complexes have the potential to provide important information on general questions regarding metal-organic complexes. They may thus act as archetype model systems for the physical behaviour of a large number of other TM complexes.

In this presentation, we will concentrate on cobalt phthalocyanine (CoPc). In this material, the Co ion appears in a divalent state with formally 7 electrons in the 3d shell. We will show results of spectroscopic measurements such as X-ray absorption spectroscopy at the Co L-edge, together with a theoretical description of the data. This approach has already proved to work successfully for transition metal oxides. Our results will clarify important aspects of the electronic structure of CoPc and shed further light on general questions regarding metal-organic complexes.

DS 18.6 Tue 14:30 Poster A

**Electronic excitation spectra of transition metal phthalocyanines** — ●ROBERTO KRAUS, MANDY GROBOSCH, and MARTIN KNUPFER — IFW Dresden, D-01069 Dresden, Germany

The electronic structure of transition metal phthalocyanine (TMPc) complexes offer valuable insight into the interaction of the metal ion with its surrounding, the organic ligand. Therefore, they represent simple model compounds for the investigation of the electronic properties of many other transition containing molecules, among them many molecular magnetic complexes. In fact, MnPc has been referred to as a typical example of a molecular magnet. Surprisingly, despite a large number of experimental and theoretical studies essential details of the electronic structure and excitations of TMPcs remained unclear, but are of tremendous importance to understand the spin and charge ground state of the enclosed transition metal ion. We present a characterization of the full electronic excitation spectra of MnPc and FePc, which have been determined using optical as well as electron energy-loss spectroscopy. We discovered low lying electronic excitations that have been observed in the past and discuss the results in view of previous theoretical work.

DS 18.7 Tue 14:30 Poster A

**Growth of CuPc thin films and metal contact formation: A photoemission study** — ●TEODOR TOADER<sup>1</sup>, GIANINA GAVRILA<sup>2</sup>, JAN IVANCO<sup>1</sup>, WALTER BRAUN<sup>2</sup>, and DIETRICH R.T. ZAHN<sup>1</sup> — <sup>1</sup>Department of Physik, Technical University Chemnitz, D-09107 Chemnitz, Germany — <sup>2</sup>BESSY GmbH, Albert-Einstein-Straße 15, D-12489 Berlin, Germany

In this study both organic/inorganic semiconductor and metal/organic film interfaces prepared under ultra-high vacuum conditions will be addressed. The growth of highly-ordered copper phthalocyanine (CuPc) films on stepped Si(111) surfaces was investigated by photoemission and near edge X-ray absorption fine structure (NEXAFS). While the

molecules take an upright orientation on hydrogen-passivated surfaces, the passivations by an ultra-thin antimony layer lead to a near lying molecular orientation. The molecular geometry in the CuPc film grown on the hydrogen-Si(111) surface was significantly influenced using a template film of 3,4,9,10-perylenetetracarboxylic dianhydride (PTCDA) deposited prior to CuPc growth. Varying molecular orientation in the CuPc films affects their electronic properties as probed via valence band photoemission spectroscopy. The interfacial chemistry and electronic structure of a metal contact, namely In-CuPc was studied during the incremental overgrowth of indium. A chemical interaction between indium and CuPc film was detected with reacted molecules tending to remain on the In surface, rather than at the In-CuPc interface.

DS 18.8 Tue 14:30 Poster A

**Spectroscopic determination of the Voigt constant of copper phthalocyanine by magneto-optical Kerr effect and ellipsometry investigations** — ●MICHAEL FRONK, DIETRICH R.T. ZAHN, and GEORGETA SALVAN — Physics Department, Chemnitz University of technology, D-09107 Chemnitz

The measurement of the magneto-optical Kerr effect (MOKE) is frequently used to monitor magnetic properties of ferromagnetic thin films during growth (e.g. [1]). MOKE spectroscopy can also be employed to determine the Voigt constant of ferromagnetic layers [2,3], if the optical constants of the involved layers are known. In this work the Voigt constant of copper phthalocyanine (CuPc) is calculated using the experimental results of polar MOKE spectroscopy and variable angle spectroscopic ellipsometry (VASE) investigations. The calculations were carried out using a three layer model air - film - substrate for normal incidence and considering the decomposition of the linearly polarised incident light into its two circularly polarised eigenmodes. The CuPc films were grown by organic molecular beam deposition in high vacuum onto silicon substrates either H-passivated or covered by native oxide. When deposited on silicon with native oxide the molecules adopt a close to standing orientation, while those grown on H-passivated substrates align with an average tilt angle of about 55° with respect to the substrate plane. This leads to significant differences in the magnitude of the Voigt constants of CuPc on the two types of substrates.

[1] M. Wahl et al., phys. stat. sol. (c) 0, 2003, 3002 [2] T. Herrmann et al., PRB 73, 2006, 134408 [3] J. Zak et al., PRB 43, 1991, 6423

DS 18.9 Tue 14:30 Poster A

**Optically detected magnetic resonance of single N-V centers in diamond for molecular spintronics** — ●JULIANE KNIEPERT, KATI HÜBENER, CHRISTOPH OELMÜLLER, and WOLFGANG HARNEIT — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

An important issue in molecular spintronics is the detection and state read-out of single spins or small spin ensembles as occur in molecular nanostructures. With their typical sensitivity of  $10^{12}$  to  $10^{14}$  spins, conventional ESR methods are not suitable for single spin detection. Optical detection (ODMR) improves the sensitivity to  $10^5$  spins. Combined with single molecule spectroscopy, the spin of an individual molecule becomes accessible.

Here, we apply the method of single spin detection to N-V centers in diamond as a read-out system for molecular spins. The nitrogen-vacancy (N-V) center consists of a substitutional nitrogen atom and an adjacent carbon vacancy. Irradiation of resonant microwaves changes the spin polarization of the ground state, resulting in a decrease of the fluorescence intensity. N-V centers are also interesting for the field of quantum information. They might be used as qubits themselves or as a read out system for other coupled spin systems e.g. organic molecules. Here we investigate the coupling of endohedral fullerenes to N-V centers. Owing to their long relaxation time endohedral fullerenes such as N@C<sub>60</sub> may be promising candidates for quantum bits.

DS 18.10 Tue 14:30 Poster A

**Optimization of spin coated thin films based on transition metal complexes towards magneto-optical applications** — ●BJÖRN BRÄUER<sup>1</sup>, TOBIAS RÜFFER<sup>2</sup>, ROBERT MOTHES<sup>2</sup>, FRANÇOIS EYA'ANE MEVA<sup>2</sup>, and GEORGETA SALVAN<sup>2</sup> — <sup>1</sup>Chemnitz University of Technology, Department of Physics, Reichenhainer Straße 70, D-09126 Chemnitz — <sup>2</sup>Chemnitz University of Technology, Department of Chemistry, Straße der Nationen 62, D-09111 Chemnitz

Coordination complexes allow the step-wise incorporation of an increasing number of transition metal ions and thereby the variation

of physical properties of the molecules. In this work a series of bis(oxamato) type transition metal complexes containing three Cu(II) ions were synthesized to investigate the influence of their central N,N'-bridge and of their terminal ligands on the magnetic and magneto-optical properties. The latter were investigated by means of magneto-optical Kerr effect (MOKE) spectroscopy. For the MOKE investigations thin films were prepared by means of spin coating (deposition) on Si wafers. This was previously demonstrated for the first time to be a promising technique for the deposition of multinuclear transition metal complexes on surfaces [1]. To improve the quality of the films in terms of homogeneity, a number of parameters had to be optimized: a) the chemical composition of the multinuclear transition metal complexes with respect to their planarity and solubility, b) the rotation speed as well as the solvent in the spin coating process. [1] B. Bräuer, D. R. T. Zahn, T. Ruffer, G. Salvan, Chem Phys Lett, 2006, 432, 1-3, 226.

DS 18.11 Tue 14:30 Poster A

**All-electron calculations of spin-polarized transport through molecules** — ●DANIEL WORTMANN, NICOLAE ATODIRESEI, and STEFAN BLÜGEL — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany

The magneto-resistive effects and coupling between an electron current and the magnetisation in planar junctions is a highly developed field and forms the basis of the field of spintronics and magnetoelectronics. The experimental and theoretical studies of related effects in molecular junctions is still at its infancy. We investigate a model system of a magnetic cobaltocene molecule sandwiched between Ni(111) surfaces by carrying out *ab initio* density functional theory (DFT) calculations of the spin-dependent transmission. The calculations of electron transport through molecules in linear response became nearly a standard for the popular gold electrodes. Our all-electron full-potential transport code is ideally suited to treat as well more complex materials and relativistic effects as well as non-collinear magnetic structures are included. Support by the DFG-SPP 1243 is gratefully acknowledged.

DS 18.12 Tue 14:30 Poster A

**Structure and morphology of thin evaporated Polycarbonate films** — ●CHRISTIAN VREE and S. G. MAYR — I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Structure formation at surfaces during thin film deposition is of great scientific interest due to the demand for smooth or regularly structured surfaces and interfaces for miniaturized functional films in science and technology. The deposition processes which govern morphology evolution during vapour deposition of polymer films are still poorly understood and need closer investigation.

Poly (Bisphenol A carbonate) (PC) thin films were deposited in a vacuum chamber on different substrates. Surface morphologies were investigated using scanning force (SFM) and scanning electron microscopy (SEM). Fourier transform infrared spectroscopy (FTIR) and size exclusion chromatography (SEC) were performed for a detailed chemical characterization. It is found, that the bond topology remains mostly unchanged, while the chain length is reduced. Evaporated films basically consist of oligomeric fractions (dimer to heptamer) of the original chains but a small amount of high molecular weight material can be observed as well. The rms-roughness decreases rapidly with film thickness on Si, SiO<sub>2</sub> and GaAs substrates, until a fully covered substrate is obtained at thicknesses as high as 30 nm. On PC substrates smooth films are observed independent of film thickness.

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DS 18.13 Tue 14:30 Poster A

**Exciton diffusion length measurements on organic thin films for the application in photovoltaic cells** — ●TOBIAS SCHUON, TOBIAS ROLLER, and JENS PFLAUM — 3. Physikalisches Institut, Universität Stuttgart, D-70550 Stuttgart

The exciton diffusion length,  $L_D$ , has an important impact on the efficiency of photovoltaic devices. Therefore the detailed knowledge of the dependence of this quantity on the structural and chemical sample properties is crucial for PV cell optimization. In this work  $L_D$  has been measured by photoluminescence quenching on layers of various materials, viz. DIP (diindenoperylene), CuPc and PTCBI, and at different thicknesses. Alternatively, we estimated  $L_D$  via the spectral PV photocurrent on the basis of a suited exciton diffusion model<sup>1</sup>. To achieve a complete set of material and device parameters, comprehensive studies by X-ray diffraction, UV-Vis spectroscopy and AFM have

been performed.

As a key result, DIP provides an exciton diffusion length in the order of 100 nm, thereby compensating for its rather weak absorption<sup>2</sup>. We related this high  $L_D$  to the fact, that DIP forms a structural phase of high crystallinity on weakly interacting substrates, with its long molecular axis preferentially oriented along the surface normal<sup>3</sup>. Furthermore, balanced electron and hole mobilities along this crystallographic direction support the application of DIP in PV devices<sup>4</sup>.

[1] A.K.Ghosh, T.Feng, J.Appl.Phys. **49**, 5982 [2] D.Kurrle, J.Pflaum, Appl.Phys.Lett. (subm.) [3] A.C.Dürr, et al., Appl.Phys.Lett. **81**, 2276 [4] A.K.Tripathi, J.Pflaum, Appl.Phys.Lett. **89**, 82103

DS 18.14 Tue 14:30 Poster A

**Nanocolloidal Scattering Particles Integrated in OLEDs** — ●BORIS RIEDEL, JULIAN HAUSS, SEBASTIAN GLEISS, ULI LEMMER, and MARTINA GERKEN — Lichttechnisches Institut, Universität Karlsruhe (TH)

Organic light emitting devices (OLEDs) combine cost-effective fabrication with large device areas. While OLEDs are starting to appear in commercial displays, they are not sufficiently bright yet for lighting applications. In current OLEDs only about 20% of the generated photons can exit the device. The rest is trapped as surface plasmon polaritons or as guided modes inside the organic layers or the substrate. We investigate the influence of nanocolloidal scattering particles on the extraction efficiency of OLEDs. These particles inhibit internal guided modes inside the OLED and thus increase the amount of extracted light. We use SiO<sub>2</sub> and ZnO dispersed in water and ethyl alcohol respectively and bring them onto the Indium Tin Oxide-anode. This modified substrate is then further processed by evaporating small molecules or by spincoating polymers. Fabricated devices are characterized electrically and optically.

DS 18.15 Tue 14:30 Poster A

***in vivo* STM-observation of the growth of 3,4,9,10 perylene tetracarboxylic (PTCDA) crystals on Si(111) 7 × 7** — ●THORSTEN WAGNER<sup>1</sup>, ROLF MÖLLER<sup>1</sup>, MASAFUMI SAKATA<sup>2</sup>, and KINGO ITAYA<sup>2</sup> — <sup>1</sup>Universität Duisburg-Essen, Fachbereich Physik, Lotharstr. 1-21, 47057 Duisburg — <sup>2</sup>Tohoku University, Department of Applied Chemistry, Sendai, Japan

We will show scanning tunnelling microscopy (STM) results on the *in vivo* observation of the growth of organic nanocrystals. 3,4,9,10 perylene tetracarboxylic dianhydride (PTCDA) was thermally evaporated onto a clean Si(111) 7×7 surface held at room temperature. A sequence of images acquired over a period of 24h shows how the unordered structure with no visible molecular resolution evolves to individual crystals which can be well characterized. The size of the crystallites (roughly 10nm by 10nm) is consistent with former thermal desorption experiments (TDS) of PTCDA on Cu(111): The number of crystals increases with the coverage. This can be related to the higher the density of nucleation centres. Between preparation and first imaging had been 12h. In addition, the formation of the crystals took place during the STM observation. Therefore we propose that the growth of the crystals is not only driven by diffusion. By operating the STM at mean current of 2pA and a bias voltage of +1.5V the tip adsorbate interaction was minimized. Anyway this small force could be enough to push and drag the molecules into the energetically preferred adsorption sites within the crystalline structures. Once the crystalline structures have been formed the images were stable and molecular resolution was possible.

DS 18.16 Tue 14:30 Poster A

**Growth monitoring of CuPc on H-Si(100) and In/CuPc interface formation Studied by Raman Spectroscopy** — MARIUS TOADER, ●PHILIPP SCHÄFER, CAMELIU HIMCINSCHI, and DIETRICH R T ZAHN — Chemnitz University of Technology, Semiconductor Physics, D-09107, Chemnitz, Germany

Copper phthalocyanine (CuPc) layers deposited under ultra high vacuum conditions using organic molecular beam deposition onto hydrogen passivated silicon H-Si(100) substrates were investigated using Raman spectroscopy. Different emission lines (from 488 nm to 676 nm) of Ar or Kr lasers were used for excitation in a backscattering geometry. *In situ* on-line growth monitoring was performed in order to determine influence of the thickness on the internal molecular vibrations. The Raman spectra, recorded in different polarization configurations, macro and micro configurations, *in situ* and *ex situ* respectively, were used to estimate the orientation of CuPc molecules in the layers. Novel devices based on organic semiconductors such as organic field effect transistors

or organic light emitting diodes require metallic contacts. Therefore, the interface between metals and organic semiconductors require special attention. *In situ* Raman scattering was thus also employed to assess the In/CuPc interface formation.

DS 18.17 Tue 14:30 Poster A

**Nanostructures to Enhance Light Extraction from OLEDs** — ●JULIAN HAUSS, SEBASTIAN GLEISS, ULF GEYER, BORIS RIEDEL, ULI LEMMER, and MARTINA GERKEN — Lichttechnisches Institut, Universität Karlsruhe, D-76131 Karlsruhe, Germany

In current organic light emitting diodes (OLEDs) only a small fraction of the generated photons can be extracted as useful light (5-20%). Besides quenching and substrate modes, guided modes in the organic layers and surface plasmons at the metal-organic interface are the main loss channels. The outcoupling of substrate modes is widely studied and established in common devices whereas for the outcoupling of guided modes and plasmons a general remedy is still lacking. We study the angular and spectral dependence of the emitted light and the ability to tailor these properties by periodic nanostructures, which scatter guided modes and surface plasmons. The investigated structures are fabricated by interference lithography, which is a promising approach to large scale and cost effective production. The experimental results are compared to numerical simulations.

DS 18.18 Tue 14:30 Poster A

**AFM Lithography on Polymer Brushes and Spin-Coated Polymer Films** — ●MICHAEL HIRTZ<sup>1</sup>, MARION K. BRINKS<sup>2</sup>, ARMIDO STUDER<sup>2</sup>, HARALD FUCHS<sup>1</sup>, and LIFENG CHI<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany — <sup>2</sup>Organisch-Chemisches Institut, Westfälische Wilhelms-Universität, Corrensstraße 40, 48149 Münster, Germany

Polymer brushes offer an interesting route to tailor surface properties [1]. Additionally it is of great interest to generate structured polymer brushes [2,3,4]. Here we present our investigation on the properties of different polymer brushes (polystyrene (PS), polyacrylate (PA) and poly(n-isopropylacrylamide) (PNIPAM)) with a thickness of 5 to 50nm grafted onto siliconoxide used as substrates for AFM lithography. In comparison to spin-coated polymer films of similar thickness, polymer brushes exhibit enhanced mechanical properties in regard to pattern fidelity, stability and resolution. The resulting patterns can be used as masks and templates for further lithographic steps.

[1] Y. Tsujii, K. Ohno, S. Yamamoto, A. Goto, T. Fukuda; Adv. Polym. Sci. (2006) 197: 1-45. [2] K.D. Dronavajjala, R. Rajagopalan, S. Uppili, A. Sen, D.L. Allara, H.C. Foley; J. Am. Chem. Soc. (2006) 128: 13040-13041. [3] Y. Tsujii, M. Ejaz, S. Yamamoto, T. Fukuda, K. Shigeto, K. Mibu, T. Shinjo; Polymer (2002) 43: 3837-3841. [4] M.K. Brinks, M. Hirtz, L.F. Chi, H. Fuchs, A. Studer; Angew. Chem. Int. Ed. (2007) 46: 5231-5233.

DS 18.19 Tue 14:30 Poster A

**Temperature dependent measurements on perylene thin-film based OTFTs** — ●CHRISTIAN EFFERTZ, MORITZ SCHAEFER, MARYAM BEIGMOHAMADI, AZADEH FARAZADI, PHENWISA NIYAMAKOM, PHILIP SCHULZ, and MATTHIAS WUTTIG — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Organic Thin-Film Transistors (OTFTs) are promising candidates for electronic applications, e.g. as an active matrix for flexible displays. Some organic materials, such as perylene, show a high field-effect mobility, comparable to hydrogenated amorphous silicon (a-Si:H). In order to describe the mechanism of charge transport, competing models, like the grain boundary model, the small polaron model and the multiple trapping and release model have been developed in the past. However, for a wide range of organic semiconductors it is not yet understood what model has to be applied. In order to gain a deeper insight into the transport mechanisms of organic materials we present temperature dependent measurements of the electronic transport in perylene-based OTFTs. The temperature range between 213K and 418K has been investigated. The TFTs were produced employing OTS and 2-propanol modified SiO<sub>2</sub> dielectric layers, on top of highly doped silicon substrates, which were used as the gate contact. Thermally evaporated gold pads acted as the contacts for the source and drain of the devices. Besides electronic measurements, additional characterization techniques, including Atomic Force Microscopy (AFM) for the surface morphology and X-Ray Diffractometry (XRD) for structural analysis of the organic layer have been employed in this investigation.

DS 18.20 Tue 14:30 Poster A

**LT-STM study of individual CuPc molecules on Cu(111)** — HATICE KARACUBAN, •JOHANNES SCHAFFERT, SASCHA KOCH, THORSTEN WAGNER, and ROLF MÖLLER — Universität Duisburg-Essen, Fachbereich Physik, Lotharstr. 1-20, 47057 Duisburg

The interface between organic semiconductors and metals plays a key role for the electronic properties and thus for their application in devices. We present a low temperature scanning tunneling microscopy and spectroscopy study of copper phthalocyanine on Cu(111). A submonolayer of CuPc was evaporated onto a clean Cu(111) single crystal at room temperature under ultra high vacuum (UHV) conditions. Previous measurements show that at room temperature single CuPc molecules are mobile on the Cu(111) surface and can not be imaged by means of STM. The presented STM measurements have been carried in UHV at temperatures below 10K. We observe CuPc adsorbed in two different geometries, as well as the equivalent sites, rotated by multiples of 60°. One of the adsorption sites leads to an apparent reduction of the molecules four-fold symmetry in the STM image. Two opposite of four benzopyrrol rings appear brighter. First spectroscopic results show, that the brighter parts also differ electronically. Furthermore, the molecules adsorbed with reduced symmetry tend to align forming chains of molecules on the Cu(111) surface.

DS 18.21 Tue 14:30 Poster A

**Ellipsometry Investigation of Pentacene Thin Films** — •MARION FRIEDRICH, DANIEL LEHMANN, FALKO SEIDEL, and DIETRICH R. T. ZAHN — TU Chemnitz, Institut für Physik, 09107 Chemnitz, Germany

Thin pentacene layers with thicknesses ranging between 20 and 150 nm were prepared by organic molecular beam deposition on native oxide covered silicon substrates. Variable angle spectroscopic ellipsometry was applied aiming at the determination of thicknesses and dielectric function of pentacene thin films. Starting with the assumption that the optical properties are the same, the optical constants of several films with different thickness were coupled and fitted together with the film thicknesses in a multi-sample analysis procedure. For thickness determination different models are employed and discussed regarding their deviation from the measurement results. Best agreement between simulation and experiment was found for a model implying uniaxial films. As a result of further detailed data evaluation in the absorbing spectral range a difference in the dielectric functions for thin and thick layers was determined.

DS 18.22 Tue 14:30 Poster A

**Spectroscopic studies of metal oxide sensitisation by self-assembling light harvesting molecules and photovoltaic applications** — •CLARE DYER-SMITH<sup>1</sup>, JENNY NELSON<sup>1</sup>, SAIF A HAQUE<sup>2</sup>, PETER MAREK<sup>3</sup>, and T SILVIU BALABAN<sup>3</sup> — <sup>1</sup>Dept of Physics, Imperial College, London SW7 2AZ, U.K — <sup>2</sup>Dept of Chemistry, Imperial College, London SW7 2AZ, U.K — <sup>3</sup>Karlsruhe Institute of Technology, Institute for Nanotechnology, Postfach 3640, D-76021 Karlsruhe

Molecular photovoltaic devices may provide a low-cost alternative to crystalline silicon solar cells with the long-term potential to displace conventional fossil fuels. Naturally occurring within green photosynthetic bacteria are metal porphyrins which self assemble to form a light harvesting antenna architecture enabling exciton transport over longer ranges. This is promising for application in organic solar cells where charge separation requires exciton diffusion to an interfacial site. Self assembly is thought to lead to improved charge transport properties and therefore improved photocurrent generation efficiency. We report studies of functionalised porphyrins acting as the donor component in molecular photovoltaic devices. We study the influence of film morphology, influenced by the porphyrin side groups, on exciton diffusion, charge separation yield and charge transport in porphyrin films on semiconducting metal oxide surfaces. Charge separation and transport properties are measured using transient optical spectroscopy and time of flight techniques and are correlated to film morphology. The structure and energetics of the donor-acceptor interface are key to maximising the potential of such systems for photovoltaic applications.

DS 18.23 Tue 14:30 Poster A

**Investigation of thermally activated charge carrier transport in thin perylene layers** — •MORITZ SCHAEFER, CHRISTIAN EFFERTZ, MARYAM BEIGMOHAMADI, PHENWISA NIYAMAKOM, AZADEH FARAHZADI, PHILIP SCHULZ, and MATTHIAS WUTTIG — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

The production of organic thin-film transistors (OTFTs) is a low cost process. Therefore, they are promising for large area TFT arrays as needed in low cost electronic paper, RFID tags, etc. [1]. Recently reported characteristics of OTFTs in terms of mobility and Ion/Ioff-ratio are similar to those of the currently used hydrogenated amorphous silicon (a-Si:H) TFTs [1]. It is now possible to produce OTFTs with a comparable high performance, but the transport phenomena in the organic layer are still not completely understood.

We present the electronic characteristics of perylene based OTFTs. Transfer and output characteristics were measured in order to determine the mobility  $\mu(T)$  and the threshold voltage  $V_T(T)$ . For this purpose, a stage was designed that can be cooled to -50°C and heat to +100°C. The active layer of the transistors was produced by vacuum thermal evaporation (VTE) via a temperature controlled substrate holder with a temperature range from -40°C to +35°C. The organic film thickness was varied between 25 nm and 500 nm. Atomic Force Microscopy (AFM) and x-ray diffraction (XRD) have been used in order to determine the crystallinity and morphology of the organic layer.

[1] D. S. Park, et. al., J. Vac. Sci. Technol. B 23(3) (2005)

DS 18.24 Tue 14:30 Poster A

**Mobile Ionic Impurities in Organic Thin Film Dielectrics for Electronic Application** — •REINHARD SCHWÖDIAUER<sup>1</sup>, MARTIN EGGINGER<sup>2</sup>, MIHAI IRIMIA-VLADU<sup>1</sup>, ANDREAS TANDA<sup>4</sup>, IRENE FRISCHAUF<sup>3</sup>, SIEGFRIED BAUER<sup>1</sup>, and SERDA SARICIFTCI<sup>2</sup> — <sup>1</sup>Soft Matter Physics, Johannes Kepler University, Altenbergerstrasse 69, 4040 Linz, Austria — <sup>2</sup>Linz Institute for Organic Solar Cells, Johannes Kepler University, Altenbergerstrasse 69, 4040 Linz, Austria — <sup>3</sup>Institute for Biophysics, Johannes Kepler University, Altenbergerstrasse 69, 4040 Linz, Austria — <sup>4</sup>Plastic Electronics GmbH, Rappesederweg 28, 4040 Linz, Austria

In the field of organic electronics organic thin film dielectrics can have a strong influence on the device performance. We present a comprehensive and comparative study of mobile ionic impurities for BCB and poly(vinyl alcohol) with traces of sodium acetate at different concentrations, ranging from below 0.004 mass% up to < 0.5 mass%. The two polymers are investigated both in a metal-insulator-metal (MIM) and a metal-insulator-(C60) semiconductor (MIS) configuration by broadband dielectric spectroscopy in the frequency- (50 \*H < f < 10 kHz), dc bias voltage (-25 V < Ubias < +25 V) and temperature (20°C < T < 120°C) domain. In addition we also present measurements on OFETs of the same material combination at different temperatures between 3°C and 60°C.

The consistent results show conclusive evidence for the impact of mobile ions in organic dielectrics for the stability and reliability of organic field effect transistors.

DS 18.25 Tue 14:30 Poster A

**Design and Performance of an Ion Beam Vacuum Deposition Apparatus Based on Electropray Ionization** — •STEPHAN RAUSCHENBACH, NICHIA THONTASEN, RALF VOGELGESANG, GIOVANNI COSTANTINI, NICOLA MALINOWSKI, and KLAUS KERN — Max-Planck-Institute for Solid State Research, Stuttgart, Germany

An electropray (ES) ion beam deposition apparatus has been developed for the high- and ultrahigh vacuum (UHV) deposition of non-volatile molecules and nanoparticles. The source employs electropray ionization to create gas phase ions, RF-quadrupoles and electrostatic ion optics for the formation and the guiding of the ion beam, differential pumping to overcome the vacuum gap to UHV and a time-of-flight mass spectrometer for in-situ characterization of the ion beam before deposition.

The ion beam is deposited on sample holders in high- and ultrahigh vacuum designed for ex-situ or in-situ analysis respectively. The parameters of the deposition, ion beam current and kinetic energy are measured and controlled before deposition, which together with the mass analysis gives complete control over the experiment. The apparatus is connected to an STM/AFM for in-situ analysis.

Time-of-flight mass spectrometry and ion beam deposition of small molecules, large biomolecules and nanoparticles is illustrated in some examples. Fluorescent molecules are used as soft landing probes, single and double layer islands of amphiphilic molecules are grown and large nanoparticles can be deposited.

DS 18.26 Tue 14:30 Poster A

**Structural, Morphological, and Optical Properties of Tetraphenylporphyrin Films on Silicon Substrates** — •SIMONA

POP<sup>1</sup>, TOBAT SARAGI<sup>2</sup>, SYLVIA WENMACKERS<sup>3</sup>, JOSEF SALBECK<sup>2</sup>, PATRICK WAGNER<sup>3</sup>, and NORBERT ESSER<sup>1</sup> — <sup>1</sup>ISAS-Institute for Analytical Sciences, Department Berlin, Albert-Einstein Str. 9, D-12489, Berlin, Germany — <sup>2</sup>Macromolecular Chemistry and Molecular Materials (mmCmm), Department of Science and Center for Interdisciplinary Nanostructure Science and Technology (CINaT), University of Kassel, Heinrich-Plett Strasse 40, D-34109 Kassel, Germany — <sup>3</sup>Hasselt University, Institute for Materials Research, Wetenschapspark 1, 3590 Diepenbeek, Belgium

Thin films of free base-meso-tetraphenylporphyrin (H2TPP) grown by organic molecular beam deposition on silicon substrates are characterized by means of spectroscopic ellipsometry, scanning electron microscopy, and atomic force microscopy techniques. The anisotropic dielectric function of H2TPP films is determined in the photon energy range from 0.73 to 5 eV. The imaginary part of the dielectric function exhibits the typical Q and Soret bands. The Q band ( $\pi$ - $\pi^*$  transition) displays the typical vibrational structure consisting of the following subbands Q<sub>x</sub>(0,0) at 1.90 eV, Q<sub>x</sub>(1,0) at 2.08 eV, Q<sub>y</sub>(0,0) at 2.2 eV, and Q<sub>y</sub>(1,0) at 2.38 eV. It is observed only for the in-plane component of the dielectric function meaning that most of the H2TPP molecules adopt a planar orientation with respect to the substrate surface. The thickness dependence of the dielectric function of the H2TPP films is additionally discussed.

DS 18.27 Tue 14:30 Poster A

**XPS and ARPES studies of azobenzene derivatives on layered materials** — ●JAROSLAW IWICKI, TILO PETER, KAI ROSSNAGEL, and LUTZ KIPP — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel, Germany

Derivatives of azobenzene with different dipole moments were deposited onto layered materials. The preparation process allows the deposition of low sublimation point molecules on a crystal surface under UHV conditions with a marginal contamination of residual gas atoms. The tube with the molecules is vacuum pumped, cooled in a nitrogen bath, heat sealed and placed in the UHV preparation chamber. The deposition process starts when the seal is broken. XPS and ARPES measurements have been carried out at the BW3 beamline at HASYLAB. XPS measurements confirm the adsorption of the azobenzene derivatives on the substrate and ARPES measurements disclose the valence electronic structure of the molecules on the crystal surface.

DS 18.28 Tue 14:30 Poster A

**Continuous Wavelength Tuning in a Wedge-Shaped Organic Microcavity Laser** — ●BERND SCHÜTTE, HANNES GOTHE, SUSANNE I. HINTSCHICH, MARKAS SUDZIUS, HARTMUT FRÖB, VADIM G. LYSSENKO, and KARL LEO — Institut für angewandte Photophysik, TU Dresden, George-Bähr-Str. 1, 01069 Dresden

Due to their broad gain spectra, lasers consisting of organic materials offer the prospect of wavelength tuning over a wide spectral range. We demonstrate a continuously tunable organic microcavity laser. Two distributed Bragg reflectors (DBRs) serve as mirrors, which are grown by reactive electron-beam evaporation. Each DBR consists of 10 alternating pairs of  $\lambda/4$  layers. A guest-host composite of Alq<sub>3</sub> and DCM is used as the gain medium. This active layer is conveniently fabricated by thermal co-evaporation, which utilizes a rotating shadow mask in order to produce a wedge shape. Wavelength tuning is achieved by ac variation of the pump beam position on the microcavity, thus changing the resonance condition in the active layer. Its wedge-shaped profile allows to continuously select any wavelength between 595 nm and 650 nm. Thus, we scan the gain spectrum of the active medium, enabling us to optimise the laser threshold. Further scope to expand this range is provided by the high chemical stability of the organic material, which allows to pump at intensities of up to three orders of magnitude beyond the lasing threshold.

DS 18.29 Tue 14:30 Poster A

**Influence of inhomogeneous broadening on the input-output characteristics of an organic microcavity** — ●SUSANNE I. HINTSCHICH, HANNES GOTHE, MARKAS SUDZIUS, HARTMUT FRÖB, VADIM G. LYSSENKO, and KARL LEO — Institut für angewandte Photophysik, TU Dresden, George-Bähr-Str. 1, 01069 Dresden

We investigate the input-output characteristics of a continuously tunable organic vertical cavity surface emitting laser (OVSEL). The microcavity consists of two distributed Bragg reflectors, which enclose an active layer of the guest:host system Alq<sub>3</sub>:DCM. The wedge-shaped geometry of this layer enables us to scan the input-output curves across

the entire gain spectrum of DCM, using a single sample. Due to the high chemical stability of the material, we can reversibly monitor the behaviour over more than 2 orders of magnitude beyond the lasing threshold at the maximum of the gain spectrum. All input-output curves deviate strongly from the standard model for homogeneously broadened emitters, which uses a single spontaneous emission factor, beta. Therefore, we take into account the inhomogeneous broadening of the organic material by introducing a distribution of beta factors. Depending on the type, width and spectral position of this distribution with respect to the cavity mode, the shape of the model curve is altered. Eventually, a Gaussian distribution with suitable parameters is used to represent the inhomogeneously broadened gain spectrum of DCM. Thus, we qualitatively model the input-output behaviour of an organic microcavity laser and demonstrate the impact of inhomogeneous broadening.

DS 18.30 Tue 14:30 Poster A

**Infrared spectroscopical studies of the evaporation, condensation and annealing process of SiO<sub>2</sub>** — ●MICHAEL MÖLLER, MARKUS KLEVENZ, and ANNEMARIE PUCCI — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

For several reasons silicon oxides are materials of persistently big interest, from astronomy to microelectronics. We studied the evaporation, condensation and annealing process of SiO<sub>2</sub> under ultra-high vacuum (UHV) conditions with *in-situ* infrared (IR) spectroscopy. All measurements were performed in an UHV chamber with base pressure below  $5 \times 10^{-10}$  mbar. First the equilibrium vapour pressure of quartz (SiO<sub>2</sub>) was determined by measuring the molecular flow from a tantalum Knudsen cell onto a quartz microbalance. Afterwards the evaporated material was deposited on different substrates with appropriate IR and thermal properties (Si, Ge, Ta). The condensation process was observed with IR transmittance (on Si, Ge) and IR reflectance spectroscopy (on Ta). The observed spectra revealed the optical properties of SiO<sub>x</sub> with the strongest Si-O stretching vibration bands at 990 and 1125 cm<sup>-1</sup>. After annealing gradually to temperatures of up to 800°C a peak shift to 1070 and 1190 cm<sup>-1</sup> was observed, respectively, before complete desorption at about 900°C occurred. The peak shifts can be explained by decomposition of the initial SiO<sub>x</sub> into Si and SiO<sub>2</sub>.

DS 18.31 Tue 14:30 Poster A

**Evaporation, condensation and annealing of forsterite studied by infrared spectroscopy** — ●MARKUS KLEVENZ<sup>1</sup>, MICHAEL MÖLLER<sup>1</sup>, MARIO TRIELOFF<sup>2</sup>, DOMINIQUE LATTARD<sup>2</sup>, and ANNEMARIE PUCCI<sup>1</sup> — <sup>1</sup>Kirchhoff-Institut für Physik der Universität Heidelberg, Deutschland — <sup>2</sup>Mineralogisches Institut der Universität Heidelberg, Deutschland

Forsterite (Mg<sub>2</sub>SiO<sub>4</sub>) is a silicate that plays a crucial role in the formation of planets and, therefore, it is of special interest in astronomy and mineralogy. Its optical phonons determine the infrared (IR) absorption and emission of protoplanetary disks. For a better understanding of the formation of the silicate compounds and the observed IR spectra, the physical and chemical properties of forsterite and later on those of other relevant silicates will be investigated in laboratory studies under well-defined similar conditions (UHV). First, the vapour pressure curves and the composition of the gas phase will be determined. This will be realized by evaporation from a Knudsen cell with defined temperatures and measuring the molecular flow onto a quartz microbalance and the composition by mass spectroscopy. Afterwards the minerals will be deposited on a substrate and characterized *in situ* by IR spectroscopy to gather information about the condensation process. Subsequently the deposited films will be annealed up to 1200 K to observe the phase transition from amorphous to crystalline *in situ* by IR spectroscopy for determining characteristic temperatures and times of the crystallization process.

DS 18.32 Tue 14:30 Poster A

**In-situ monitoring of electrochemically prepared organic films** — ●KARSTEN HINRICHS<sup>1</sup>, SIMONA SILAGHI<sup>1</sup>, MATTHIAS INTELMA<sup>2</sup>, KATY RODENKO<sup>1</sup>, NORBERT ESSER<sup>2</sup>, and JÖRG RAPPICH<sup>1</sup> — <sup>1</sup>ISAS - Institute for Analytical Sciences, Department Berlin, Albert-Einstein-Str. 9, 12489 Berlin, Germany — <sup>2</sup>Hahn-Meitner-Institut Berlin GmbH, Abt. Silizium-Photovoltaik, Kekuléstr. 5, 12489 Berlin, Germany

In-situ investigations of Si surfaces during electrochemical modification can elucidate reaction schemes and process steps. Such studies provide information about intermediate surface species during processing and

species post-formed after the treatment in solution. Grafting of organic molecules is a widely used process to functionalize the silicon surface with respect to nanopatterning, passivation or change in electronic properties. In the presented work infrared spectroscopic ellipsometry (IRSE) and reflectance anisotropy spectroscopy were applied for in-situ monitoring of the electrochemical growth of thin organic films at the silicon-liquid interface. In particular the spectra taken during the growth of a few nm thick polypyrrole and nitrobenzene films will be discussed.

DS 18.33 Tue 14:30 Poster A

**Molecular orientation in Au-molecular layer-GaAs diodes studied by IR ellipsometry** — •DANA MARIA ROSU<sup>1</sup>, AARON TRIONFI<sup>3</sup>, JULIA HSU<sup>3</sup>, KAREN KAVANAGH<sup>4</sup>, ULLRICH SCHADE<sup>2</sup>, NORBERT ESSER<sup>1</sup>, and KARSTEN HINRICH<sup>1</sup> — <sup>1</sup>ISAS - Institute for Analytical Sciences, Department Berlin, Albert-Einstein-Str. 9, 12589 Berlin, Germany — <sup>2</sup>Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung mbH, Albert-Einstein-Str. 15, 12589 Berlin, Germany — <sup>3</sup>Sandia National Laboratories, Albuquerque, New Mexico 87185- 1120 — <sup>4</sup>Kavanagh Lab, Dept. of Physics, Simon Fraser University, 8888 University Dr., Burnaby, BC, V5A 1S6, Canada

Synchrotron mapping IR ellipsometer at BESSY[1] was used for investigation of molecular orientation and lateral homogeneity in different organic-GaAs hybrid diodes with a lateral resolution below 1 mm<sup>2</sup>. Organic films on GaAs and Au are compared, the organic layer being either octanedithiol (C8DT), or hexadecanethiol (C16MT). Analysis of the CH<sub>2</sub> stretching vibrations provides informations on the structure of the main backbone, while the CH<sub>3</sub> stretching bands is giving informations about the structure and orientation of the end group of the molecules. The bands for C16MT on GaAs show a different orientation in comparison with C8DT. Evaluation of measured spectra with optical models enables spectra interpretation.

[1] M. Gensch, N. Esser, E. H. Korte, U. Schade, K. Hinrichs, *Infrared Physics and Technology* 49 (1-2) (2006) 39-44

DS 18.34 Tue 14:30 Poster A

**Infrared Synchrotron Mapping Ellipsometry of biomolecular thin films** — •DANA MARIA ROSU<sup>1</sup>, ULLRICH SCHADE<sup>2</sup>, NORBERT ESSER<sup>1</sup>, and KARSTEN HINRICH<sup>1</sup> — <sup>1</sup>ISAS- Institute for Analytical Sciences, Department Interface Spectroscopy, Albert-Einstein-Str. 9, 12489 Berlin, Germany — <sup>2</sup>BESSY GmbH, Albert-Einstein-Str. 15, 12489 Berlin, Germany

The IR synchrotron ellipsometer at BESSY II, for the mid infrared range, enables investigation of samples with monolayer sensitivity and a lateral resolution below 1 mm<sup>2</sup>. Being equipped with a mapping table [1], the set-up allows the investigation of heterogeneous organic thin films. In cooperation with Sentech Instruments the IR synchrotron mapping ellipsometer was upgraded with a rotating retarder. In the recent years IR ellipsometry has been applied for structural analysis of thin organic films [2]. Results from mapping ellipsometry of biosensors [3] and molecular monolayers, with thicknesses between 2 nm and 100 nm, will be presented. Evaluation of measured spectra with optical models gives informations about thickness, homogeneity and orientation of the molecules on the substrates.

[1] M. Gensch, N. Esser, E. H. Korte, U. Schade, K. Hinrichs, *Infrared Phys. and Technol.* 49(1-2)(2006) 39-44

[2] K. Hinrichs, M. Gensch, N. Esser, *Appl. Spectrosc.* 59 (2005) 272A-282A

[3] K. Hinrichs, M. Gensch, N. Esser, U. Schade, J. Rappich, S. Kröning, M. Portwich, R. Volkmer, *Anal. and Bioanal. Chem.* 387(5)(2007) 1823-1829

DS 18.35 Tue 14:30 Poster A

**Online monitoring of the surface properties of mixed polymer brushes via in-situ infrared ellipsometry** — •DENNIS AULICH<sup>1</sup>, IGOR LUZINOV<sup>2</sup>, OLHA HOY<sup>2</sup>, LEONID IONOV<sup>3</sup>, SERGIY MINKO<sup>4</sup>, KLAUS-JOCHEN EICHHORN<sup>3</sup>, MANFRED STAMM<sup>3</sup>, NORBERT ESSER<sup>1</sup>, ULLRICH SCHADE<sup>5</sup>, and KARSTEN HINRICH<sup>1</sup> — <sup>1</sup>ISAS, Department Berlin, Albert-Einstein-Str. 9, 12489 Berlin — <sup>2</sup>Clemson University, Clemson, SC 29634-0971, USA — <sup>3</sup>IPF Dresden, Hohe Str. 6, 01069 Dresden — <sup>4</sup>Clarkson University, Potsdam, New York 13699, USA — <sup>5</sup>BESSY II, Albert-Einstein-Str. 15, 12489 Berlin

As a new type of functional surfaces, mixed polymer brushes offer a wide range of applications due to the possibility of changing the surface properties by external stimuli such as pH, solvent, light or electric field [1, 2]. Two different mixed polymer brushes were prepared using two subsequent "grafting to" procedures (a mixed P2VP-PAA and a mixed

PEG-PAA/PS brush, each with 50/50 composition). The composition of the film was analyzed quantitatively by VIS-IR-ellipsometry. The in-situ-characterization was done by polarization dependent infrared (IR) ellipsometry in single reflection geometry both in the laboratory and in the synchrotron IR beamline at BESSY II. Exposure of the samples to different solutions at varying pH led to structural and chemical changes. Repeating cycles of systematic change of pH led to strong, reversible switching of the brush which was analyzed online via the component specific vibrational bands of the polymers.

References: [1] S. Minko et al., *Macromol. Rapid Commun.* 22(3): 206, 2001; [2] L. Ionov et al., *Langmuir* 21(19): 8711, 2005

DS 18.36 Tue 14:30 Poster A

**Study of perylene films by Fourier transform infrared spectroscopy** — •LI DING, KOSTIANTYN V. SHPORTKO, PHILIP SCHULZ, AZADEH FARAHZADI, and MATTHIAS WUTTIG — Institute of physics (IA), RWTH Aachen University, 52056, Aachen, Germany

Organic semiconductors has attracted considerable attention recent years due to their potential application in electronic devices. Fourier transform infrared spectroscopy (FTIR), as a useful tool to study vibrational properties of molecules, contains information on the molecular orientation in films [1]. Since the molecular stacking has a significant impact on the electronic and optical properties of films, it is of great interest to understand the molecular orientation in thin films [2].

Thermally evaporated perylene films are grown on a silver layer deposited on glass substrates. Infrared reflectance spectra of perylene films on Ag/glass have been measured with the incident angle from 20° to 70°. The change of absorption intensities at different incident angles indicates that the average orientation of perylene molecules on Ag/glass tends to be perpendicular to the substrate surface. XRD pattern shows that thick perylene films are highly crystalline. We have compared the absorption frequencies and intensities of perylene film with those of isolated molecules. Some new frequencies are seen in the spectrum of crystalline perylene film, which are attributed to the dimer structure in the crystalline phase.

[1] D. L. Allara, J. D. Swalen, *J. Phys. Chem.* 86, 2700 (1982).

[2] K. Akers, R. Aroca, A. Hor, R.O. Loutfy, *J. Phys. Chem.* 91, 2954 (1987).

DS 18.37 Tue 14:30 Poster A

**Tip-Enhanced Optical Microscopy of Single-Walled Carbon Nanotubes** — •CARSTEN GEORGI<sup>1</sup>, HUIHONG QIAN<sup>1</sup>, NEIL ANDERSON<sup>2</sup>, LUKAS NOVOTNY<sup>2</sup>, and ACHIM HARTSCHUH<sup>1</sup> — <sup>1</sup>Department Chemie und Biochemie & CeNS, Ludwig-Maximilians-Universität München, Germany — <sup>2</sup>University of Rochester, The Institute of Optics, Rochester, New York 14627, USA

Optical Microscopy with nanoscale spatial resolution is an essential technique for the detection and characterization of individual nanoobjects and nanostructured materials. We use the field enhancement in the proximity of a laser-illuminated sharp metal tip to locally excite and probe the optical response of nanoscale systems. In particular, we image the vibrational and electronic properties of single-walled carbon nanotubes with a spatial resolution of down to 10nm, limited only by the tip diameter [1,2]. Local perturbations along an individual nanotube, as well as energetic coupling between different nanotubes can thereby be directly observed, revealing the interaction of phonons and excitons with the nanotube structure and its environment.

[1] A. Hartschuh et al., *Nano Lett.* 5, 2310 (2005)

[2] N. Anderson et al., *Nano Lett.* 7, 577 (2007)

DS 18.38 Tue 14:30 Poster A

**Vibrational Study of Free-Base Tetraphenylporphyrin Films** — •SIMONA DORINA POP, DANA MARIA ROSU, KARSTEN HINRICH<sup>1</sup>, and NORBERT ESSER — ISAS-Institute for Analytical Sciences, Department Berlin, Albert-Einstein Str. 9, D-12489, Berlin, Germany

The vibrational structure of the vacuum deposited free-base meso-tetraphenylporphyrin (H<sub>2</sub>TPP) films on silicon substrates is investigated by infrared spectroscopic ellipsometry. The dielectric function of the H<sub>2</sub>TPP films is determined in the mid-infrared energy range. The H<sub>2</sub>TPP films exhibit a uniaxial structure in agreement with the results obtained by spectroscopic ellipsometry performed in the visible energy range. The orientation of the H<sub>2</sub>TPP molecules on silicon substrates as well as the thickness dependence of the IR dielectric function are analyzed. The assignment of the observed vibrational bands is performed with the help of density functional theory method.

DS 18.39 Tue 14:30 Poster A

**Application of Raman Spectroscopic Techniques in the Characterization of Nanostructured Semiconductors and Semiconductor Microstructures** — •DIMITRA PAPADIMITRIOU — National Technical University of Athens, Faculty of Applied Sciences, Department of Physics, GR-15780 Athens, Greece

Applications of Raman spectroscopic techniques in basic and applied research studies are reviewed. Emphasis is given to the characterization of structural phases, phase-transformation, and nanometric scale effects in nanostructured semiconductors by Raman and the validation of strain-stress effects in semiconductor microstructures by micro-Raman Spectroscopy. In particular: a) applications of combined Raman scattering and photoluminescence emission techniques in the de-

termination of the pressure dependence of the energy band-gap and the transformation pressure of nanocrystalline (porous) silicon under high hydrostatic pressure are presented [1], b) applications of the Raman selection rules in the structural characterization of light emitting silicon quantum wires are discussed [2], and c) the relevance of micro-Raman techniques for the characterization of elastic strain in porous silicon microstructures is demonstrated [3].

References: [1] D. Papadimitriou, Y.S. Raptis and A.G. Nassiopoulou, *Phys. Rev. B* 58(21), 14089, (1998). [2] D. Papadimitriou and A.G. Nassiopoulou, *J. Appl. Phys.* 84(2), 1059 (1998). [3] D. Papadimitriou, C. Tsamis, A. Nassiopoulou, *Sensors and Actuators B: Chemical* 103(1-2), 356 (2004).