CPP 12: Poster: Nanoparticles and Composite Materials

Time: Monday 17:30–19:30

CPP 12.1 Mon 17:30 Poster C

Experimental Observation of the wetting property of homopolymer on a grafted polymer on a curved substrate — •CHANG JONG KIM¹, MARKUS MAZUROWSKI², JUN YU LI¹, MARKUS GALLEI², KATRIN SONDERGELD², HENRICH FRIELINGHAUS³, MATTHIAS REHAHN², and BERND STÜHN¹ — ¹Experimental Condensed Matter Physics, TU Darmstadt — ²Ernst-Berl-Institute for Technical and Macromolecular Chemistry, TU Darmstadt — ³Jülich Centre for Neutron Science, Forschungszentrum Jülich GmbH

The wetting property of homopolymer on a grafted polymer on a nanoparticle surface is greatly influenced by the ratio of the molar mass of the polymer on the surface (N) and the matrix polymer (P). Grafting density and the ratio of the length of grafted polymer (\mathbf{R}_q) to the radius of a core (R_c) may play an important role in the wetting property as well. The change of the wetting property, the wettingdewetting transition, is therefore expected to be induced by a combination of three parameters: P/N, R_g/R_c ratio and grafting density. In our experiment, Polystyrene (PS) was grafted from the surface of nanoparticles (silica and deuterated PS). These particles were then dispersed in deuterated PS matrices and measured by Small Angle X-ray Scattering (SAXS) and Small Angle Neutron Scattering (SANS). P/N ratio was varied from <1 to $\gg1$ and R_g/R_c ratio was tuned by using two different molar masses of the grafted chain onto which the same core was used. In particular the analysis of the SANS results allows to determine thickness and conformation of the polymer brush on the curved substrate.

CPP 12.2 Mon 17:30 Poster C

Electrochemical Approach to Control CdSe/ZnS Quantum Dot Fluorescence — •DAVID PLOTZKI, NICOLE AMECKE, and FRANK CICHOS — Molecular Nanophotonics Group, University of Leipzig

The fluorescence behaviour of colloidal semiconductor nanocrystals can be tuned by adjusting the electric conditions of their close environment. We aim to electrochemically manipulate the charge concentration on the nanocrystal surfaces in order to alter the occupancy of trap states. Recent research indicates that such surface traps strongly influence nonradiative decay channels.

We investigate single colloidal CdSe/ZnS Quantum Dots on ZnOcoated ITO surfaces. Using a confocal microscope setup with the ability to study lifetimes and spectra, we explore the fluorescence behaviour under specific electrochemical potentials.

From ensemble as well as single QD measurements we find potential ranges where the nanocrystal fluorescence is either enhanced or suppressed, accompanied by a decrease or increase of the total nonradiative decay rate. Additionally, sudden potential changes cause a delayed fluorescence response. These results hint at a rearrangement of the occupancy of trap states.

CPP 12.3 Mon 17:30 Poster C

Influence of gold nanoparticle distributions on SERS enhancement factors — •THOMAS SANDER¹, HONGMEI LIU², XINPING ZHANG², and PETER J. KLAR¹ — ¹I. Physikalisches Institut, Justus-Liebig-Universität Giessen — ²College of Applied Sciences, Beijing University of Technology

Surface enhanced Raman spectroscopy (SERS) of metallic nanostructured substrates can provide Raman intensities increased by several orders of magnitude making even the detection of single molecules possible. Two different mechanisms contribute to the enhancement of the Raman signals: The electromagnetic enhancement is due to excited surface plasmons of the metal structure causing locally increased electromagnetic fields. The chemical enhancement is due to various effects, e.g. the chemical interaction between the molecules and the surface.

Here we present Raman spectra of rhodamine 6G on gold nanostructures fabricated by solution processible gold nanoparticles on Si substrates. The properties of the gold nanostructures can easily be varied by annealing at different temperatures as shown by AFM and SEM. A gold coordinate grid on the Si substrate allows one to correlate the recorded Raman spectra with the AFM and SEM measurements. Thus the influence of the gold nanoparticle distribution on the signal enhancement is accessible in detail. Raman spectra will be discussed with respect to different excitation lasers and polarizations as well as the achieved enhancements with respect to the local environment of the gold nanoparticles. COMSOL simulations of the enhancement factors will be compared with the experimental results.

CPP 12.4 Mon 17:30 Poster C Optical switchable properties of polymer-carbon-nanotubes nanocomposites based on photochromic molecules — \bullet VIKTOR SCHNEIDER¹, THOMAS STRUNSKUS¹, MADY ELBAHRI², and FRANZ FAUPEL¹ — ¹Technische Fakultät der Uni Kiel, Institut für Materialwissenschaft-Materialwissenschaft-Nanochemistry and Nanoengineering

Photochromic molecular switches are a class of organic molecules that allow a reversible control over the molecular structure or the molecular dipole moment with light. This attributes provide the possibility of photoswitching of bulk properties of composite materials like electrical conductance or dipole moment. In this work, azobenzene based chromophores were incorporated into polymer-carbon-nanotubes nanocomposites, and the photoswitching properties were investigated in a self made electro-optical measuring station. The changes in electrical resistance by illumination with ultraviolet (360 nm) and blue light (480 nm) were measured. For the multi wall carbon nanotubes, switching amplitudes of several percent were achieved, while single wall carbon nanotubes showed even changes up to 30 percent in resistance. The switching and conductance change mechanisms will be discussed.

CPP 12.5 Mon 17:30 Poster C Synthesis and characterization of silica-encapsulated Ni nanorods — •Florian Krämer, Andreas Tschöpe, and Rainer Birringer — Universität des Saarlandes, Saarbrücken

Ni nanorods are uniaxial ferromagnetic particles which can be used in nanorheology to probe local viscoelastic properties of soft matter. The present study is focused on the encapsulation of the nanorods by a silica layer which provides a well-defined interface for subsequent surface functionalization. Alumina templates with hexagonally arranged pores were synthezised by two step anodization of aluminum. The alumina-layer was separated by a voltage reversal technique. The barrier oxide at the pore-bottom was dissolved by chemical etching resulting in free-standing mesoporous membranes with completely open pore morphology. The whole surface of the membrane including the porewalls was coated with a thin silica layer by atomic layer deposition. Ni nanorods were synthesized by direct current electro-deposition of Ni into the pores. The filled templates were characterized by static magnetization measurements revealing a coercivity of $\mu_0 H_C = 56 \text{ mT}$. Afterwards the rods were released from the template by dissolution of the alumina in NaOH. Transmission electron microscopy revealed a rod diameter of 60 nm and a thickness of the silica layer of 3 nm. The anisotropic optical properties of the rods which are the physical basis for magneto-optical rheometry, were investigated with regards to the influence of the silica layer and the size of the nanorods.

CPP 12.6 Mon 17:30 Poster C Sol-Gel Templated Zinc Oxide Films for Applications in Hybrid Photovoltaics — •ERIK BRADEN, KUHU SAKAR, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany In recent years a broad field of research concerning hybrid solar cells has been developed as they show a high potential to become an impor-

has been developed as they show a high potential to become an important source of green energy. Hybrid solar cells consist of an inorganic electron acceptor and an organic hole-conductor. In the present study, zinc oxide is utilized as the inorganic material in the form of nanostructures. Zinc oxide (ZnO) nanostructures are synthesized on silicon substrates forming grid-like morphology. The synthesis is done by using a sol-gel mechanism coupled with an amphiphilic diblock copolymer poly(styrene-block-4-vinyl pyridine) P(S-b-4VP), acting as a template. The morphology is synthesized by using zinc acetate dihydrate (ZAD) as a suitable commercial ZnO precursor on silicon (100) substrates using different deposition techniques. This involves spin-coating, spraycoating, dip-coating, blade-coating and solution casting. It is tried to produce a homogenous film with a certain thickness range between 300 nm and 500 nm which is expected to be most favorable for the solar cell performance. The influences of the different coating techniques on the morphology are investigated by optical microscopy, scanning electron microscopy (SEM) and atomic force microscopy (AFM). The thickness is measured with white light interferometry and height profilometry. An overview about the surface roughness of the films is obtained via atomic force microscopy (AFM).

CPP 12.7 Mon 17:30 Poster C

Thermal and mechanical properties of styrene butadiene rubber/alumina nanocomposites — •RYMMA SUSHKO, JÖRG BALLER, MARLENA FILIMON, and ROLAND SANCTUARY — Laboratory for the Physics of Advanced Materials, University of Luxembourg, 162a avenue de la Faiencerie, L-1511, Luxembourg

SBR is a rubber material with high technical relevance. In order to enhance the mechanical properties of the rubber we dispersed inorganic nanoparticles in the polymer matrix. By doing so, the properties of a given composite can be tuned either by changing the nanoparticle concentration or by modifying the surface properties of the fillers. Both interventions have indeed the potential to take influence on the structure and properties of the interphases emerging between the fillers and the polymer matrix. In this contribution we report on the glass transition behavior of SBR/alumina nanocomposites when the concentration and surface properties of the alumina nanoparticles are changed. We also discuss the influence of the fillers on the shear stiffness of the rubber material. The samples were investigated by TMDSC and DMA methods. TMDSC investigations shed light on a surprising behavior of the glass transition temperature when the nanoparticle concentration is changed: at low filler contents the glass transition temperature Tg passes through a minimum. While further increasing the nanoparticle content Tg increases to finally saturate at high concentrations. One of the main DMA results is that increasing of the alumina concentration induces a quasi-solid-like frequency-independent response of the nanocomposites in the low frequency regime.

CPP 12.8 Mon 17:30 Poster C $\,$

Novel approach for the rapid thermal processing of polymermetal composites using 2.45 GHz microwave radiation — •ANDREAS WURM¹, RADU NICULA², KOTARO ISHIZAKI², MANUELA STIR², SEBASTIEN VAUCHER², EVGENY ZHURAVLEV¹, and CHRISTOPH SCHICK¹ — ¹University of Rostock, Institute of Physics — ²Swiss Federal Laboratories for Materials Science and Technology - Empa, Advanced Materials Processing

In contrast with traditional polymer melt-processing methods, new opportunities for improved material properties are sought by various R&D and industrial groups through the use of powder processing technologies, in particular for polymer-matrix composites. For example, in the field of new biomaterials for acetabular cup prosthetics, UHMWPE composites comprising AlCuFe quasicrystalline (QC) particles were shown to exhibit significantly improved wear loss properties compared to pure UHMWPE or Al2O3/UHMWPE composites, without loosing the excellent biocompatibility of the UHMWPE matrix. Further improvement of the wear resistance of such composite materials is nowadays sought in the better anchoring of the metal particles to the polymer matrix. Towards this objective, a novel rapid thermal processing approach is proposed that mainly exploits the selective absorption of microwave field energy by the metal particle constituent of the composite material.

CPP 12.9 Mon 17:30 Poster C Fast Spectral Analysis of Quantum Dot Blinking —

•CLEMENS GÖHLER, CORNELIUS KRASSELT, and CHRISTIAN VON BORCZYSKOWSKI — Chemnitz University of Technology, Institute of Physics, Germany

While investigating individual semiconductor nanocrystals (quantum dots, QDs) using single molecule techniques, photoluminescence intermittency (blinking) can be observed. This means emission is temporarily suppressed under constant excitation. This behaviour can be explained by a trapping model, assuming electron and hole to be localised in trap-states in QD interfaces or the environment [1].

It has been shown that a two-level-system with on- and off-intensity does not exactly describe the blinking process since experiments imply the existence of intermediate intensities as well [2]. According to the trapping model, this may refer to a hole-trapping mechanism. Additionally, the localised charge will influence the recombination process due to the quantum-confined Stark effect, resulting in spectral shifts within the photoluminescence.

In our experiments we investigate this spectral diffusion in relation

to the intermediate intensities. Confocal microscopy is used to detect photoluminescence light from single ZnS/CdSe QDs. Moreover, emission light is separated onto two individual photodiodes by passing a dichroic beam splitter and the intensity levels are determined from recorded photon arrival times using a Change-Point-Algorithm.

F. Cichos, C. von Borczyskowski, M. Orrit: COCIS 12(2007), 272.
R. Schmidt, C. Krasselt, C. von Borczyskowski: Chem. Phys. 406(2012), 9.

CPP 12.10 Mon 17:30 Poster C $\,$

Morphology studies for titania nanoparticle based hybrid solar cells — •STEPHAN PRÖLLER, VOLKER KÖRSTGENS, and PETER MÜLLER-BUSCHBAUM - TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany Thin films containing titania nanoparticles have a variety of applications. For applications in photovoltaics a high absorption coefficient and a large surface area are desirable. Blends of organic and inorganic semiconductors are denoted as hybrid solar cells. Those hybrid solar cells combine the advantages of inorganic semiconductors with the film-forming polymer. Properties of inorganic nanoparticles are size tunability, high absorption coefficients and high mobilities. We use nanoparticles as acceptors in polymer-titania hybrid solar cells. Furthermore, we investigate the influence on the performance of solid-state dye sensitized solar cells based on ruthenium dye and spiro-OMeTAD as hole transport material. The thin films are prepared via spin-coating and solution casting, respectively. The surface structure is investigated with SEM. Thickness and structure of the layer are studied with XRR, the optical properties with UV/Vis spectroscopy and the efficiency of the different solar cells is measured under AM 1.5 conditions.

CPP 12.11 Mon 17:30 Poster C Thin films of sponge-like titania nanostructures with controllable thickness — •LIN SONG, MARTIN A. NIEDERMEIER, and PE-TER MÜLLER-BUSCHBAUM — TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany

Titania nanostructures have a huge application potential, e.g. in photovoltaics, photocatalysis and gas sensing. For all these applications, a high surface area is important. Sponge-like titania nanostructures are especially promising due to their morphology with a high surface area and an interconnected network. The titania nanostructures are prepared from block copolymer templating in combination with sol-gel chemistry. The templated titania sol-gel is deposited on a substrate by spin-coating, via calcination the polymer template is combusted and nanostructured crystalline titania thin films are obtained. Additionally, the sol-gel approach allows for a control of the film thickness. The surface morphology is investigated with scanning electron microscopy (SEM) and optical microscopy (OM), the optical properties and the film thickness are probed with UV/Vis spectroscopy and ellipsometry.

CPP 12.12 Mon 17:30 Poster C Ultrafast Spectroscopy of excitonic states in an individual CdSe nanowire — •THORSTEN SCHUMACHER^{1,2}, HARALD GIESSEN², and MARKUS LIPPITZ^{1,2} — ¹Max Planck Institute for Solid State Research, Stuttgart — ²4th Physics Institute, University of Stuttgart

We investigate the spectrally resolved ultrafast carrier dynamics of excitonic states of a single CdSe nanowire at room temperature. The transient absorption spectra show characteristic short and long living effects that we attribute to a highly excited electron-hole plasma and excitonic state bleaching. We discuss both phenomena and show a very good agreement between the detected bleaching signal and the dipole allowed excitonic transition energies, calculated by a six band-effective mass model. Furthermore we extract the lifetime of various transitions and set them in comparison to the corresponding photoluminescence response. Here we obtain hints on radius fluctuations within a single wire leading to an enhanced probability of spontaneous emission at these large radius defects.

CPP 12.13 Mon 17:30 Poster C Analyzing the electrical properties of percolating carbon nano-tubes or nano-fibers in composite-materials — •MICHAEL KONTER¹, PABLO CARBALLEIRA², BERND WETZEL², and ROLF PELSTER¹ — ¹Fachrichtung 7.2 Experimentalphysik, Universität des Saarlandes, Saarbrücken, Germany — ²Institut für Verbundwerkstoffe GmbH, Kaiserslautern, Germany

We compare different types of composite materials containing carbon nano-fibers (CNF) or carbon nano-tubes (CNT) with fillings ranging from 0-2%. These were dispersed in an epoxy resin either with a three roll calendar device or with a torus mill laboratory mixing device. After polymerization solid samples are obtained that were characterized via temperature dependent dielectric spectroscopy (10 Hz - 2 GHz, 40 K - 290 K). For samples above the percolation threshold ($f_c = 0, 08vol.\%$) we observe a broad polarization process, that is correlated with the dc-conductivity. An effective medium analysis reveals several intrinsic parameters. Here we discuss (i) the ratio of the inter-fiber or intertube contact resistance to the intrinsic resistance, $R_{contact}/R_{carbon}$ and (ii) the product of percolation strength and intrinsic CNT or CNF conductivity, $C \cdot \sigma_{carbon}$, as well as its activation energy. The data reveals the quality of the inter-fiber contacts and thus reflects differences in the sample preparation.

CPP 12.14 Mon 17:30 Poster C Structure-Property relationships of Nanocomposites Based on Polylactide and Layered Double Hydroxides — •JING LENG¹, PURV PUROHIT¹, DE-YI WANG^{2,3}, and ANDREAS SCHOENHALS¹ — ¹BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany — ²Madrid Institute for Advanced Studies of Materials, C/Eric Kandel 2, 28906 Getafe, Madrid, Spain — ³Center for Degradable and Flame-Retardant Polymeric Materials (ERCEPM-MoE), College of Chemistry, Sichuan University, Chengdu 610064, China

Abstract: Polymer based nanocomposites prepared by melt blending of synthesized NiAl layered double hydroxides (NiAl-LDH) and polylactide (PLA) were investigated by combination of differential scanning calorimetry (DSC), small- and wide-angle X-ray scattering (SAXS and WAXS) and broadband dielectric spectroscopy (BDS). In the case of NiAl-LDH based nanocomposites the degree of crystallinity at first increases and then decreases as a function of LDH concentration. By extrapolation a limiting concentration of NiAl-LDH ca.15% where the crystallization of PLA is completely suppressed by the nanofiller. The dielectric spectra of the nanocomposites show several relaxation processes related to dynamic glass transition and localized fluctuations were identified and analyzed in detail to understand the morphology. The results of the PLA based nanocomposites with NiAl-LDH as nanofillers were further compared with PLA based nanocomposites with MgAl-LDH as nanofillers.

CPP 12.15 Mon 17:30 Poster C

Ultrafast strain-mediated response of functionalized polyelectrolyte nanolayers — •STEFFEN MITZSCHERLING — Universität Potsdam

We prepared layered functional nanostructure samples by spin-assisted layer-by-layer deposition of polyelectrolytes. In analogy to our previous study on spherical gold nanoparticles we show that gold nanorods exhibit even larger spectral shifts and amplitude variations when their dielectric environment is modified.[1,2]

We use the plasmon resonance of the metallic particles to detect ultrashort strain pulses travelling through polymeric layer structures. These hypersound waves are generated by excitation of azobenzenecontaining layers. We characterize the strain pulse by ultrafast broadband Brillouin-scattering [3] in order to derive conclusions on the actuation and nonlinear propagation in such complex polymeric nanolayer systems.

 $[1]{\rm Kiel}$ et al., Langmuir, 28, 4800 (2010).

[2]Kiel et al., Langmuir, 26, 18499 (2012).

[3]Bojahr et al., Physical Review B, 86, 144306 (2012).

CPP 12.16 Mon 17:30 Poster C

Analysis of Particle-Particle Interaction Potentials in Aqueous Nanoscale Systems — •JULIAN SCHULZE¹, MICHAEL PAULUS¹, JOHANNES MÖLLER¹, METIN TOLAN¹, and ROLAND WINTER² — ¹Fakultät Physik / DELTA, Technische Universität Dortmund, 44221Dortmund, Germany — ²Fakultät Chemie, Technische Universität Dortmund, 44221 Dortmund, Germany

In previous studies small angle X-ray scattering (SAXS) was used to study the interaction potential of proteins in aqueous solution under the influence of varying conditions such as pressure, temperature or further cosolvents. A non-linear correlation between the strength of the protein-protein interaction and hydrostatic pressure was found with a minimum at 2 kbar. Adding salts led to a linear increase of the attractive part of the interaction potential, while adding Trimethlyaminoxid (TMAO) causes a shift of the minimum to higher pressures. In the presented work the pressure dependent behavior of the interaction potential of nano particles is determined by SAXS. Furthermore, the pressure dependent structure of the solvent is explored by wide angle X-ray scattering (WAXS). Spherical nanoparticles are used because their structure factor is easy to model. Besides the WAXS data is not influenced by the scattering signal from the complex inner structure of proteins, so that changes of the water structure factor can be determined.

CPP 12.17 Mon 17:30 Poster C Spectroscopic Ellipsometry of Anisotropic Nanocomposites —•JOHANNES F. H. RISCH¹, BASTIAN BESNER², MARYAM HASHEMI², MATTHIAS SCHWARTZKOPF¹, ADELINE BUFFET¹, BERIT HEIDMANN¹, GERD HERZOG¹, VOLKER KÖRSTGENS³, EZZELDIN METWALLI³, JAN PERLICH¹, ANDRE ROTHKIRCH¹, MONIKA RAWOLLE³, KAI SCHLAGE¹, PETER MÜLLER-BUSCHBAUM³, RALF RÖHLSBERGER¹, RAINER GEHRKE¹, MICHAEL A. RÜBHAUSEN², and STEPHAN V. ROTH¹ — ¹DESY, Hamburg, Germany — ²Uni. Hamburg, Institut für Angewandte Physik, Hamburg, Germany — ³TU München, Physik Department E13, Garching, Germany

Optical anisotropic thin films have a wide field of application like antenna, sensors or LEDs. Vacuum sputter deposition, which is commonly used in industry has been proven a reliable method for preparing thin films. Glancing angle deposition (GLAD) [1] of gold on top of a colloidal array of polystyrene nanospheres was used to create anisotropic optical properties in nanocomposite thin films. Using spectroscopic ellipsometry, we investigated the change of optical properties caused by asymmetric deposition of gold clusters. Since commercial standard software does not enclose applicable fitting models, a new analyzing software is developed fulfilling the complex demands to model anisotropic media. In order to extract the optical response of each active layer, a systematic sample analysis comprising the measurements of single components of GLAD samples was performed. As a result, an energy depending change of azimuthal symmetry is observed. [1] Gonzalez-Garcia et al., ChemPhysChem 11, 2005 (2010)

CPP 12.18 Mon 17:30 Poster C Spectroscopic Ellipsometry of Anisotropic Nanocomposites —•JOHANNES F. H. RISCH¹, BASTIAN BESNER², MARYAM HASHEMI², MATTHIAS SCHWARTZKOPF¹, ADELINE BUFFET¹, BERIT HEIDMANN¹, GERD HERZOG¹, VOLKER KÖRSTGENS³, EZZELDIN METWALLI³, JAN PERLICH¹, ANDRE ROTHKIRCH¹, MONIKA RAWOLLE³, KAI SCHLAGE¹, PETER MÜLLER-BUSCHBAUM³, RALF RÖHLSBERGER¹, RAINER GEHRKE¹, MICHAEL A. RÜBHAUSEN², and STEPHAN V. ROTH¹ — ¹DESY, Hamburg, Germany — ²Uni. Hamburg, Institut für Angewandte Physik, Hamburg, Germany — ³TU München, Physik Department E13, Garching, Germany

Optical anisotropic thin films have a wide field of application like antenna, sensors or LEDs. Vacuum sputter deposition, which is commonly used in industry has to be proven a reliable method for preparing thin films. Glancing angle deposition (GLAD) [1] of gold on top of a colloidal array of polystyrene nanospheres was used to create anisotropic optical properties in nanocomposite thin films. Using spectroscopic ellipsometry, we investigated the change of optical properties caused by asymmetric deposition of gold clusters. Since commercial standard software does not enclose applicable fitting models. a new analyzing software is developed fulfilling the complex demands to model anisotropic media. In order to to extract the optical response of each active layer, a systematic sample analysis comprising the measurements of single components of challenging GLAD samples was performed. As a result, an energy depending change of azimuthal symmetry is observed. [1] Gonzalez-Garcia et al., ChemPhysChem 11, 2005 (2010)

 $\begin{array}{c} \text{CPP 12.19} \quad \text{Mon 17:30} \quad \text{Poster C} \\ \textbf{OLED structures utilizing silicon nanoparticles} & -- \mbox{ Hans} \\ \text{VOLKER STEGEMANN}^1, \bullet \text{JENS THEIS}^1, \mbox{ AXEL LORKE}^1, \mbox{ and HART-MUT WIGGERS}^2 & -- \mbox{ }^1 \mbox{Fakultät für Physik and CENIDE, Universität Duisburg-Essen} \\ \mbox{ Duisburg-Essen } & -- \mbox{ }^2 \mbox{Institut für Verbrennung und Gasdynamik and CENIDE, Universität Duisburg-Essen} \\ \end{array}$

We have fabricated electroluminescence devices based on silicon nanoparticles (Si-NP) and conducting polymers. The Si-NPs have been synthesized from the gas phase in a low-pressure microwave plasma using SiH₄ as a precursor.

Two different sample designs were developed and characterized. For the first kind of samples, the NPs were embedded in a layer structure consisting of hole-conducting and electron-conducting polymers. For electrical contact an evaporated silver film was used as cathode and a transparent indium tin oxide (ITO) coated glass slide as anode. For the second sample structure, the NPs were embedded between two electrodes in a conducting polymer matrix. Here ITO/glass was used as anode. For the cathode different metals have been employed to investigate their influence on the luminescence.

Carrying out electroluminescence measurements, we obtain visible light emission for both sample structures. The spectra showed two broad bands which could be identified by additionally performed PLmeasurements as the emission from the Si-NPs and the polymers, respectively.

CPP 12.20 Mon 17:30 Poster C

Photoluminescence of CdSe, Au and Hybrid Nanoparticle Systems — •DANIEL BRAAM¹, ZHENG MA¹, PIN-WEN WANG^{1,2}, JENS THEIS¹, GÜNTHER M. PRINZ¹, PHILIPP WAGENER³, STEPHAN BARCIKOWSKI³, and AXEL LORKE¹ — ¹Fakultät für Physik and CENIDE, University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany — ²Harvard School of Engineering and Applied Sciences Pierce Hall 29 Oxford Street Cambridge, MA 02138, USA — ³Fakultät für Chemie and CENIDE, University of Duisburg-Essen, Universitätsstraße 7, 47057 Duisburg, Germany

Gold and Gold/Silver nanoparticles were fabricated with laser ablation and characterized with SEM, TEM, UV/VIS and photoluminescence measurements. They show a large size distribution and agglomeration, as well as a broad PL signal, which results from the decay of a particle plasmon within the model of Dulkeith et al [1]. Continuous excitation with a 405nm diode laser steadily shifts the peak wavelength to lower energies and reduces the intensity, which regenerates to some extend after exposure. In a second step we examine the interaction between metal and semiconductor nanoparticles by adding CdSe/ZnS quantum dots to the Au and Au/Ag NP solutions. First spectrum and peak analysis show mixed emission, which can be explained by a simple superposition of the Au and the CdSe NP PL. No indication of interaction between metallic and semiconductor nanoparticles is observed in the emission energies, presumably due to insufficient mixing, leading to a large distance between both components.

[1] E. Dulkeith et al., PRB **70**, 205424 (2004)

CPP 12.21 Mon 17:30 Poster C

AFM and physicochemical characterization of Upconversion Nanoparticles — •Heba S. Mohamad¹, Peter Nestler¹, Harm Wulff¹, Stefanie Perfahl², Patrick Bednarski², and Christiane A. Helm¹ — ¹Inst. für Physik, Uni Greifswald, D-17487 Greifswald — ²Inst. für Pharmazie, Uni Greifswald, D-17487 Greifswald Recently, the development of upconversion nanoparticles (UCNPs) for fluorescence imaging and drug delivery monitoring attracted attention. For biological labeling, cancers diagnosis and detection, NaYFH₄O: Yb,Er is a promising candidate. The sequential absorption of two or more photons in the near infrared (NIR) leads to an emission in the visible range. The NaYFH₄O:Yb,Er nanoparticles aggregate in water. Therefore their surface is modified using different approaches. Since the upconversion depends strongly on the crystallographic structure of the UCNPs (either cubic or hexagonal), the ratio of both species within an adsorbed layer needs to be optimized to improve the upconversion property. Main goals of this investigation are formation of homogenous and well distributed UCNPs layers, to examine the upconversion properties.

To determine the size of UCNPs, Atomic Force Microscopy (AFM) is used. The crystalline structure is characterized by the X-ray diffraction (XRD) pattern, to correlate optical with crystallographic properties. The absorption properties are determined with UV-Vis absorption spectroscopy. With a 980 nm laser excitation source the upconverting properties are investigated.

CPP 12.22 Mon 17:30 Poster C $\,$

Correlation of optical characteristics of gold nanoparticle-DNA networks with size and internal structure — •MALTE LINN¹, ANNE BUCHKREMER², JAN TIMPER³, THOMAS ECKERT⁴, WALTER RICHTERING⁴, JOACHIM MAYER³, GERO VON PLESSEN¹, and ULRICH SIMON² — ¹Inst. of Physics (IA), RWTH Aachen University — ²Inst. of Inorganic Chemistry, RWTH Aachen University — ³Central Facility for Electron Microscopy, RWTH Aachen University — ⁴Inst. of Physical Chemistry, RWTH Aachen University

The application of nanoplasmonic materials relies on the fabrication of metallic nanostructures with well defined sizes and geometries. By mixing different ratios of DNA-functionalized gold nanoparticles (AuNPs), various kinds of DNA-AuNP networks can be tailored. The size and internal structure of these networks determines their optical properties, due to interparticle coupling. The networks are thermally and photothermally addressable and therefore interesting for possible applications in the fields of drug release or gene regulation. In this work, we analyze the size and internal structure of DNA-AuNP networks by combining optical extinction spectroscopy, dynamic light scattering, small angle X-ray scattering, in situ-TEM measurements and generalized Mie calculations. Using these techniques, we determine the different interparticle distances in the networks. For small networks, they are consistent with a center-shell geometry.

CPP 12.23 Mon 17:30 Poster C Broadband Dielectric Spectroscopy and Rheology on Polyisoprene Silica Nanocomposites — •Adrian Hamm¹, Gerald J. Schneider², Lutz Willner¹, Wim Pyckhout-Hintzen¹, Reiner Zorn¹, and Dieter Richter¹ — ¹Jülich Centre for Neutron Science JCNS-1, Jülich, Deutschland — ²Jülich Centre for Neutron Science JCNS-FRM-II, Garching, Deutschland

Even though polymer nanocomposites have been playing a crucial role in our daily life for many years, the microscopic origin of the material properties is not fully understood. Therefore, we performed dielectric spectroscopy and rheology experiments on simple model-like polyisoprene silica nanocomposites.

In general, the response of polymer melts to an external perturbation, such as an electric field or a mechanical stress, causes a signal that depends on the sample and on the method. Even in case of identical samples, the measured relaxation function can be different and thereby reveal different details on the molecular origin of the measured values. In our contribution, we demonstrate how to ascribe the different relaxation functions measured by rheology and by broadband dielectric spectroscopy in nanocomposites to the different origins inherent with the different methods.

CPP 12.24 Mon 17:30 Poster C Computational Simulation of Molecular Motors — •ABBAS ALI DEHGHAN BAGHI — Ruhr-University Bochum, Bochum, Germany

We have used molecular mechanics simulations based on Force Field methods to study the molecular systems which would be able to perform a rotation motion. The research intends to understand the fundamental principles of these molecular motions. We used classical simulations methods by using TINKER package to optimize such molecular systems and do the basic analysis of these systems. But, we have checked our results with quantum chemistry calculations methods. The *ab initio* electronic structure calculations were performed using the TURBOMOLE package where DFT calculations have been done on the B97-D (GGA) level with Triple-Zeta Valence Plus Polarization (TZVPP) basis sets and the dispersion correction in the package is based on the atom-pair wise DFT+D2 level. We have focused on the binding energy of the molecular structures as a key factor to our analysis on both classical and quantum chemistry methods. We are interested in supramolecular motors whose stator and rotor are not covalently attached to each other, but are held mechanically and act like a "Ball and Bowl" which rotate without axle to each other. The fullerene C_{60} corresponds to the ball and is referred as a guest and Tribenzotriguinacen molecule corresponds to the Bowl and is referred as a host. We have investigated that the interaction between the host and the guest is solely due to dispersive interactions which has been certified by a negligible charge transfer from the host to the guest C_{60} upon binding and such systems are among physisorption systems.

CPP 12.25 Mon 17:30 Poster C Surfactant modified silica particles at the air/water interface — •ADRIAN CARL, ANNE BANNUSCHER, and REGINE VON KLITZ-ING — TU Berlin, Straße des 17. Juni 124, Institut für Physikalische Chemie, Stranski Laboratorium

The combination of nanoparticles and suitable surfactants has been shown to increase aqueous foam stability compared to the same system without nanoparticles. The origin of the increased stability is not fully resolved, yet. Unmodified, hydrophilic nanoparticles show no attachment to the water/air interface. On addition of surfactant, the particles are rendered hydrophobic and adsorb to the interface. In equilibrium, a specific surface coverage is obtained. At the interface, a comparatively rigid particle layer, withstanding compression, is formed. The location within the interface is governed by the particle's wetting properties which are expressed by the contact angle.

We conduct x-ray reflectivity (XRR) measurements to characterize the equilibrium state of the adsorbed particle layer. The results are related to surfactant adsorption isotherms and the adsorption kinetics are obtained from dynamic surface tension measurements.

CPP 12.26 Mon 17:30 Poster C Erbsenzählerei ? Wieso Nanopartikel gezählt werden müssen, und wie das gehen kann. — •WENDEL WOHLLEBEN, JULES MIKHAEL und VOLODYMYR BOYKO — BASF SE, Material Physics

Aufgrund der EU regulatorischen Definition von *Nanomaterial* müssen zehntausende von partikulären Produkten auf ihre Anzahlverteilung der enthaltenen Nanopartikel untersucht werden. Das trifft die Physik und Messtechnik unvorbereitet. Mit Ringversuchen und gezielten Validierungen wurden die Grenzen der Anwendbarkeit von etablierten und neuen Methoden ausgelotet.[1] Einzelpartikel- und Fraktionierungs-Methoden wie NTA, EZS, FFF, AUC haben Vorteile bei den inhomogenen, polymorphen, durch Wechselwirkung mit ihrer Umgebung veränderten Materialien[2,3], können aber oft Partikel unter 20nm oder über 1mum nicht erfassen. Streu-Methoden wie DLS oder SLS scheitern an der Polydispersität, andere wie AFM und TEM-Tomographie sind statistisch nur marginal belastbar. Eine regelrechte Messstrategie muss mit 1D, 2D und 3D Nanomaterialien validiert werden, bevor unbekannte Proben als regulatorisches Nanomaterial identifiziert werden können.

[1] J. Nanopart. Res. (2012) DOI 10.1007/s11051-012-1300-z

[2] Nanoscale (2012) DOI: 10.1039/c2nr32711b

[3] ACS Nano 6 (2012) 4603

 $CPP \ 12.27 \quad Mon \ 17:30 \quad Poster \ C$ Microscopic Investigation of Polymer Chain Dynamics in Nanocomposites with Strong Attractive Interaction — •THOMAS GLOMANN¹, GERALD J. SCHNEIDER², JÜRGEN ALLGAIER², and DIETER RICHTER² — ¹Jüllich Centre for Neutron Science & Institute for Complex Systems, Forschungszentrum Jülich, 52425 Jülich, Germany — ²Jülich Centre for Neutron Science, Forschungszentrum Jülich, Outstation at FRM 2, Lichtenbergstraße 1, 85747 Garching, Germany

The mechanical properties of polymer based nanocomposites are essentially determined by surface interactions between the chains and filler particles. In particular the strong hydrogen bonding interaction energy causes dynamic adsorption of chain segments on hydrophilic surfaces which is often reported to yield an immobilized layer of mostly suppressed or "glassy" dynamics.

Using high-resolution quasi-elastic neutron scattering techniques we found experimental evidence for highly flexible chain dynamics within the adsorbed layers on both the large and local length scale. We present results of neutron spin-echo and time-of-flight measurements on PEO-Silica model systems where the interaction energy was tuned using differently terminated polymers.

CPP 12.28 Mon 17:30 Poster C

In-situ Synthesis of Semiconductor Nanoparticles Decorating Tubular J-aggregates — •YAN QIAO, FRANK POLZER, HOLM KIRMSE, EGON STEEG, STEFAN KIRSTEIN, and JÜRGEN P. RABE — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

Organic/inorganic hybrid nanomaterials, that combine the strengths of the individual organic and inorganic materials while compensating for their deficits, have recently attracted more and more attention. Quasi one-dimensional (1-D) nanomaterials, such as wires and tubes, have been intensively investigated owing to the benefit of dimensionality on electronic and optical properties [1]. Based on our previous results on silver [2], this work focuses on the fabrication of quasi 1-D organic/inorganic hybrid nanostructures consisting of nanotubular J-aggregates self-assembled from amphiphilic cyanine dyes, and semiconductor nanoparticles such as CdS decorating the surface of the nanotubes. Electrostatic interaction between the negative surface potential of the aggregates and the Cd2+ leads to the enrichment of Cd2+ within the ionic double layer close to the aggregate surface. Addition of thioactamide leads to the formation of CdS nanocrystals with diameters less than 6 nm. With investigation of cryo-TEM and UV-Vis spectroscopy, It is found that CdS nanoparticles are exclusively formed at the surface of the aggregates. This opens a route to the formation of efficiently electronically coupled organic/inorganic systems.

[1] Y. N. Xia et al., Adv. Mater. 2003, 15, 353.

[2] D. M. Eisele et al., J. Am. Chem. Soc. 2010, 132, 2104.

CPP 12.29 Mon 17:30 Poster C

Tuning the electronic properties of the CuInS2 nanoparticles for application in hybrid solar cells — \bullet Rany Miranti¹,

CHRISTOPHER KRAUSE¹, DOROTHEA SCHEUNEMANN¹, JOHANNES NEUMANN², DANIELA FENSKE², JOANNA KOLNY-OLESIAK¹, HOLGER BORCHERT¹, and JÜRGEN PARISI¹ — ¹Univ. of Oldenburg, Dept. of Physics, Energy and Semiconductor Research Laboratory, 26111 Oldenburg, Germany — ²Fraunhofer IFAM, Marie-Curie-Str.1-3 26129 Oldenburg, Germany

CuInS2 (CIS) is one interesting material in solar cell applications because of the wide absorption range extending into the NIR and a lower toxicity. Despite much research in the CIS-based solar cells, the performance of CIS nanocrystal (NC) solar cells remains low so far. In case of CIS/polymer bulk heterojunction solar cells the surface properties of the NCs are one important issue in this field. Modifying these surface properties is a promising method to influence the performance of the solar cells. Varying Cu to In precursor ratio in the synthesis leads to differences in the Cu and In concentrations in the CIS NCs' surfaces. CIS NCs prepared with Cu excess seem to accept more electrons than those with In excess. In the present work, CIS NCs were synthesized and characterized by XRD and TEM. Furthermore, we studied the composition of the NCs and the ligand shells by EDX and TGA, as well as the I-V characteristics in the hole and electron only devices. The influence of the Cu to In precursor ratio during the synthesis of CIS NCs on the performance of solar cells will also be discussed.

CPP 12.30 Mon 17:30 Poster C Gold nanoparticles decorated with oligo(ethylene glycol) thiols: surface charges, and interactions with proteins in solution — •Fajun Zhang¹, Moritz Schollbach¹, Felix Roosen-RUNGE¹, MAXIMILIAN W. A. SKODA², ROBERT M. J. JACOBS³, and FRANK SCHREIBER¹ — ¹IAP, Universität Tübingen — ²STFC, ISIS, Rutherford Appleton Laboratory, UK — 3 University of Oxford, UK We have studied the stability of OEG SAM decorated gold nanoparticles (AuOEG) and their interactions with proteins in solutions using DLS and zeta-potential measurements. We show that AuOEG particles carry a low net negative charge and are stable under a wide range of experimental conditions [1]. When mixed with proteins, negatively charged proteins do not adsorb to the colloid surface. However, with positively charged protein (lysozyme), zeta-potential values increase with protein concentrations and lead to a charge inversion, indicating adsorption of lysozyme to the colloid surface. The colloidal solutions become unstable near zero charge. Washing protein-bound colloids by centrifugation can remove only part of the adsorbed lysozyme. The effective charge inversion and rather strongly bound lysozyme on the colloid surface suggest that in addition to the charges formed at the SAM-water interface, there are defects on the surface of the colloid, which are accessible to the proteins [2]. The results of this study of surface charge, and stability shed light on the interaction with proteins of SAM coated AuNPs and their applications. [1] F. Zhang, et al. J. Phys. Chem. A 2007, 111, 12229. J. Phys. Chem. C 2009, 113, 4839. [2] M. Schollbach, et al. 2012, Submitted

CPP 12.31 Mon 17:30 Poster C Optical and electrical properties of novel C_{60}/C_{1-3} carbon cluster material. — •DMITRY STRELNIKOV and MANFRED M. KAPPES — KIT, Institute of Physical Chemistry II, Fritz-Haber-Weg 2, 76131 Karlsruhe

 C_{60} and C_1, C_2, C_3 clusters were co-deposited on SiO₂ substrate under high-vacuum conditions. Produced films were annealed to various temperatures up to 1200 K. Raman, UV-Vis spectra were measured ex-situ to characterize electronic and structural properties of the obtained carbon material. 4-point resistivity measurements were also performed. The obtained material may be interesting for carbon-based electronics.

CPP 12.32 Mon 17:30 Poster C Fluorine patterning in C2Fx determined by solid-state NMR and DFT — •ANASTASIA VYALIKH and ULRICH SCHELER — IPF Dresden

A combination of solid-state NMR and DFT has been used to elucidate the structure of room-temperature synthesized graphite fluorides C2Fx intercalated with acetonitrile. 13C MAS NMR spectra confirm that all carbon sheets have been subjected to fluorination irrespective of the fluorination degree. However, the presence of graphite-like domains has been evidenced in the material with a low fluorination degree. By combining the 19F MAS NMR with DFT calculations, we demonstrate that all kinds of fluorine decoration patterns (isolated, end chain, midchain, cyclic and branched CF groups as well as infinite CF arrays and peripheral CF2 defects) may exist in the low-temperature produced graphite fluorides. Analysing the data with different degree of fluorination, an evolution of fluorine patterns was proposed, involving CF

chain formation and propagation towards the increasing chain length.