

## CPP 8: Poster: Nanoparticles and Composite Materials

Time: Monday 17:30–20:00

Location: Poster A

CPP 8.1 Mon 17:30 Poster A

**Dielectric investigation of nanocomposites based on Polystyrene and Polyhedral Oligomeric Silesquioxanes**

— ●MOHAMMAD MIR MOHAMMAD SADEGHI, PURV PUROHIT, ANNABELLE BERTIN, MARTIN BÖHNING, and ANDREAS SCHÖNHALS — BAM Federal Institut for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany

Enhancement of polymer properties by use of different types of nano-sized fillers has attracted a growing attention of scientists recently. Polymer based nanocomposites have shown improvement in properties as compared to conventional scaled composites because of the length scale of interaction between the nanofillers and the polymer matrices. Efforts are made to fully understand the relationship between structure and properties of such polymer based nanocomposites. Nanocomposites of Polystyrene as matrix and MethacrylPOSS (MPOSS) as the nanofiller and crosslinker were synthesized. For preparation of the nanocomposites, different concentrations of MPOSS have been applied. In order to investigate the structure-property relationships of the nanocomposites, several methods such as dielectric relaxation spectroscopy, fourier transform infrared spectroscopy, differential scanning calorimetry, and thermal gravimetric analysis have been employed.

CPP 8.2 Mon 17:30 Poster A

**Maghemite nanoparticles in thin block copolymer films**— ●YUAN YAO<sup>1</sup>, EZZELDIN METWALI<sup>1</sup>, VOLKER KÖRSTGENS<sup>1</sup>, EVA HERZIG<sup>1</sup>, WEIJIA WANG<sup>1</sup>, ADELIN BUFFET<sup>2</sup>, STEPHAN V. ROTH<sup>2</sup>, MATTHIAS OPEL<sup>3</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany — <sup>2</sup>HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany — <sup>3</sup>Walther-Meißner-Institut, Walther-Meißner-Str. 8, 85748 Garching, Germany

Maghemite nanoparticles embedded inside a polymer matrix mark a new class of hybrid materials which have attracted high interest. The control of the alignment of the maghemite nanoparticles within the polymer matrix is essential for producing well-aligned highly-oriented metal-polymer nanocomposites. The alignment of maghemite nanoparticles in poly(styrene-*b*-methyl methacrylate) diblock copolymer films is investigated. Two different sizes of maghemite nanoparticles are used: One is below and the other one above the critical particle size of the single magnetic domain. Films are prepared by solution casting within an external magnetic field. The morphology and inner nano-structure of the resulting hybrid films is studied as a function of the external magnetic field strength and for different concentrations of maghemite nanoparticles. The structure characterization of the films is based on optical microscopy, atomic force microscopy, and grazing incidence small-angle x-ray scattering. In addition, the magnetic properties are measured for different temperatures and compared with theoretical predictions.

CPP 8.3 Mon 17:30 Poster A

**Structure-property relationship of Nanocomposites based on Polylactide and Carbon nanotubes**

— ●PURV PUROHIT and ANDREAS SCHÖNHALS — BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany

The concept of biodegradable plastics is of considerable interest with respect to solid waste accumulation. Among numerous kinds of degradable polymers, polylactic acid sometimes called polylactide, an aliphatic polyester and biocompatible thermoplastic, is currently a most promising and popular material with the brightest development prospect and is considered as the \*green\* eco friendly material. So nanocomposites based on PLA and CNT can prove to be a promising class of material.

Nanocomposites with different concentrations of CNT in PLA were prepared via melt blending. The properties are studied using combination of various characterization techniques such as differential scanning calorimetry (DSC), small and wide angle X-ray scattering (SAXS & WAXS) and dielectric relaxation spectroscopy (DRS).

CPP 8.4 Mon 17:30 Poster A

**Diffraction around a Single Heated Nanoparticle**

— ●MARKUS SELMKE, MARCO BRAUN, and FRANK CICHOS — Universität Leipzig, Exp. Phys. I, molecular nanophotonics

Within the growing field of nano-sciences a fruitful new domain of metal nano-particles (NPs) has emerged: NPs of different shapes and composition have been used as markers, field-/ temperature-sources and sensors in many studies. Their unique and tunable absorptive properties are utilized in single particle photothermal (PT) detection which overcomes the scattering cross-section limitation of regular dark/wide-field and confocal microscopes. It is based on the (lock-in-)detected intensity-modulation of a probing laser beam caused by a particle-centered refractive index profile which is generated almost instantaneously through the absorption of a modulated heating laser. Thereby, even single molecules may be detected and a dispersion-like signature of the signal is obtained, which is what one would expect for a lens affecting the propagation of the gaussian probe beam. So far, no model exists which is able to describe the axial shape of the detected signal, nor does a quantitative theory for the signal magnitude exist at all. This gap, which so far separates this ultra-sensitive imaging technique from a quantitative tool, was bridged by the development of quantitative theories which are able to reproduce the full body of observed phenomena. One of them, the diffraction model presented here is shown to be particularly intuitive, quantitative and simple.

CPP 8.5 Mon 17:30 Poster A

**Growth of silver nanowires within nanotubular J-aggregates**

— ●EGON STEEG, HOLM KIRMSE, JÜRGEN P. RABE, and STEFAN KIRSTEIN — Institut für Physik, Humboldt-Universität zu Berlin

It was demonstrated earlier that ultrathin but long Ag nanowires with a diameter less than 7 nanometers and a length exceeding micrometers can be fabricated by reduction of silver salt using uniform nanotubular J-aggregates of amphiphilic cyanine dyes as template [1]. Here we report on the growth mechanism of these Ag wires as revealed by transmission electron microscopy. The growth of the wires is photo-initiated by short illumination with blue light and is terminated at different time steps by removing Ag<sup>+</sup> ions upon adding NaCl to the solution. In this case the Ag<sup>+</sup> ions react with the Cl<sup>-</sup> ions to form AgCl nanocrystals. At times shorter than 2 hours, small and well separated fragments of silver wires are found along the aggregates with a broad length distribution in the range of ten to hundred nanometers. At times later than 2 hours, homogeneous wires are found with lengths of microns filling almost the entire aggregates. By high-resolution TEM one finds microcrystalline domains with sizes up to 100 nm. These findings show that the growth of the wires starts independently at distinct nucleation centers and proceeds to fill the entire aggregate. This growth process must be supported by transport of Ag<sup>+</sup> ions through the tubular wall membrane.

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

CPP 8.6 Mon 17:30 Poster A

**Interfacial Properties of Grafted Nanoparticle Based Nanocomposites**— ●MATHIAS MEYER<sup>1,2</sup>, EIKE HÜBNER<sup>3</sup>, WIM PYCKHOUT-HINTZEN<sup>1,2</sup>, JÜRGEN ALLGAIER<sup>1,2</sup>, and DIETER RICHTER<sup>1,2</sup> — <sup>1</sup>Jülich Centre for Neutron Science, Forschungszentrum Jülich GmbH, Jülich, Germany — <sup>2</sup>Institute for Complex Systems, Forschungszentrum Jülich GmbH, Jülich, Germany — <sup>3</sup>Institut für Organische Chemie, Technische Universität Clausthal, Clausthal, Germany

Though nanocomposites with their astonishing properties are of great interest for research and industry, microscopic details of the polymer-interface have been scarcely investigated. Therefore a model system basing on grafted silica nanoparticles is designed and studied. From TEM, SANS and SAXS experiments, particle sizes and their distribution were determined independently. They also reveal a core-shell-like structure of the non-grafted particles which has been neglected in literature so far. The influence of the grafting density and the chain length and type of the graft as well as of the dispersing medium were investigated in terms of a polydisperse core-shell-type model. Our experimental results are compared to multiscale simulations within an EU FP7 project (NanoModel), focussing on the radial density profile of the polymer shell. Due to our newly developed 'grafting to' approach a labelling of the grafted chains is now possible, which allows for the first time to investigate the chain conformation in the shell.

CPP 8.7 Mon 17:30 Poster A

**Microscopic Characterization of Nanocomposites Featur-**

**ing Attractive Polymer-Particle Interactions** — •THOMAS GLOMANN<sup>1</sup>, GERALD SCHNEIDER<sup>2</sup>, WIM PYCKHOUT-HINTZEN<sup>1</sup>, JÜRGEN ALLGAIER<sup>1</sup>, and DIETER RICHTER<sup>1</sup> — <sup>1</sup>Jülich Centre for Neutron Science (JCNS-1) & Institute for Complex Systems (ICS-1), Forschungszentrum Jülich GmbH, D-52425 Jülich — <sup>2</sup>Forschungszentrum Jülich GmbH, JCNS am FRM II, Lichtenbergstr. 1, 85747 Garching

Attractive surface interactions between the particle and the polymer phase result in a layer of adsorbed chains on the particle surface which greatly influences e.g. the viscoelastic properties of the nanocomposite.

Poly(alkylene oxide)s (PAO)s mixed with bare silica nanoparticles are ideal model systems to gain microscopic insights on the role of surface interactions in nanocomposites. Strong attractive interactions are present between the OH-groups on the silica surface and the oxygen in the polymer backbone due to hydrogen bonding. Different sets of low and high molecular weight samples were prepared by solution blending of silica nanoparticles with appropriate mixtures of protonated and deuterated chains.

We present first results of our investigations of the microscopic chain structure and chain dynamics in the presence of adsorbing surfaces by means of using small-angle neutron scattering and neutron spin-echo spectroscopy.

CPP 8.8 Mon 17:30 Poster A

**Continuous flow-through synthesis of prismatic silver nanoparticles in micro fluid segment sequences for possible SERS application** — •ANDREA KNAUER<sup>1</sup>, ANDREA CSAKI<sup>2</sup>, WOLFGANG FITZSCHE<sup>2</sup>, and JOHANN MICHAEL KÖHLER<sup>1,2</sup> — <sup>1</sup>University of Technology Ilmenau, D-96893, Ilmenau, Germany — <sup>2</sup>Institute of Photonic Technology (IPHT) Jena, D- 07745, Jena, Germany

Non-spherical noble metal nanoparticles of gold and silver are of great interest due to their size- and shape-dependent plasmonic absorption in the long wavelength range. The spectral position of the in-plane dipole resonance wavelength can be tuned by the lateral length of the nanoparticles. It was expected that the homogeneity of nucleation and particle growth is influenced by the mixing speed due to the strong effect of reactant concentrations on the nucleation rate. Thus, the particle quality should improve, if high mixing rates under micro continuous-flow conditions and narrow residence time distributions are applied. The segmented flow technique was applied in order to combine a fast mixing by a segment-internal convection and a narrow residence time distribution. From the first synthesis step, homogeneous Ag seeds are obtained. In the second synthesis procedure, silver ions and a reducing agent are dosed into micro droplets containing Ag seeds in order to form silver nanoprisms, which display high size homogeneity. The presented technique can be adapted to synthesize colloidal solutions with tuneable particle sizes. Thus, the long-wavelength absorption can be shifted in a range between 520 and 1000 nm.

CPP 8.9 Mon 17:30 Poster A

**Metal nanoparticle affected molecular emission: A density matrix approach** — •YUAN ZHANG<sup>1,2</sup>, YAROSLAV ZELINSKY<sup>1</sup>, and VOLKHARD MAY<sup>1</sup> — <sup>1</sup>Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, D-12489 Berlin, Germany — <sup>2</sup>University of Science and Technology Beijing, XueYuan Road 30, 100083 Beijing, P. R. China

To compute the emission spectrum of a molecule metal nanoparticle complex a full quantum mechanical description of the system is presented. Based on a density matrix approach the computation accounts for intramolecular vibrational relaxation, nanoparticle plasmon damping, coupling to the photon field, and a non-perturbative consideration of the molecule nanoparticle interaction [1]. The latter is responsible for a remarkable plasmon induced decrease of the molecular radiative life-time. We investigate this life-time shorting in its effect on the time- and frequency resolved emission spectrum of the molecule nanoparticle complex. By including optical excitation of the system transient and steady-state spectra are presented.

[1] Y. Zelinsky and V. May, Chem. Phys. Lett. **511**, 372 (2011).

CPP 8.10 Mon 17:30 Poster A

**Time-resolved measurements on electron beam exposed Upconversion phosphors** — •MANUELA REITZIG<sup>1</sup>, THOMAS HÄRTLING<sup>1</sup>, ANTON MAYER<sup>2</sup>, and JÖRG OPITZ<sup>1</sup> — <sup>1</sup>Fraunhofer Institute for Nondestructive Testing IZFP, Dresden, Germany — <sup>2</sup>GigaTag GmbH, Oberpfaffenhofen, Germany

Since the development of infrared and Upconversion lasers and opti-

cal amplifiers, Upconversion materials have attracted significant attention. For several interesting applications trivalent rare-earth ions such as Er<sup>3+</sup>, Tm<sup>3+</sup>, Yb<sup>3+</sup> and Y<sup>3+</sup> were doped as luminescent centers in certain hosts such as oxysulfides and fluorides. Their unique optical properties depend on the host material and the dopant lanthanide ion and its concentration. Here we report on observation of alterations of the optical Up- and Downconversion properties due to electron beam treatment and discuss possible changes respective the crystalline and electronic structure of the material. The luminescence lifetime lasts for a few milliseconds and becomes sizably faster after electron beam treatment. We achieved to build up an optical set up we are able to obtain the decay time and spectrally resolved. With these observations we envisage a new application field for Upconversion phosphors, namely the optical, hence fast and contactless testing of e-beam irradiation. To this end rare-earth-based phosphors are placed as marker material inside or on a product packaging material. Upon electron irradiation the marker material changes its luminescent properties as a function of applied energy dose.

CPP 8.11 Mon 17:30 Poster A

**Stabilizing Foams with Nanoparticles** — •ADRIAN CARL and REGINE VON KLITZING — Stranski-Laboratorium, Institute of Chemistry, Berlin Institute of Technology, Strasse des 17. Juni 124, 10623 Berlin, Germany

In the recent years, it has been shown by various groups that nanoparticles can be used to stabilize aqueous and oily foams [1]. The stabilization can be achieved without the use of surfactants. By appropriate tuning of the nanoparticle wetting properties, the adsorption of particles to the interface can be strongly favored. Due to the irreversible attachment of nanoparticles at the air/water interface, the surface elasticity and rheology of those foams is remarkably different from foams stabilized by surfactants. Various approaches can be used to hydrophobize particles. In addition, the process of foam formation has a strong impact on the resulting foam structure. An optimum in foamability of particle solutions is found for intermediate wettability.

Our work focuses on basic understanding of how the surface properties of modified silica nanoparticles influence their wetting behavior. Nanoparticles with varying degrees of functionalization and the resulting foams were characterized by scattering and microscopic techniques to gain insight into the governing principles of this comparatively young research field.

[1] A. Carl, R. von Klitzing, Angew. Chem., Int. Ed. **2011**, *50*, 11290-11292

CPP 8.12 Mon 17:30 Poster A

**Photothermal spectroscopy studies of quantum dots in liquid crystals** — •ANDRÉ HEBER, MARTIN PUMPA, MARKUS SELMKE, MARCO BRAUN, NICOLE AMECKE, and FRANK CICHOS — Molecular Nanophotonics, University of Leipzig, Leipzig, Germany

Fluorophores have played an important role for single-molecule techniques but they suffer from bleaching which limits the observation time. Metallic nanoparticles can overcome this limitation. They constantly absorb light that is dissipated into the environment as heat. This temperature increase results in a change of the refractive index around the particle being detected by a probing laser beam. Usually gold nanoparticles are used as they have a large absorption cross section as compared to the 100-fold smaller one of quantum dots. We try to compensate this by observing quantum dots in a liquid crystal (5CB) slightly below the phase transition temperature from the nematic to the isotropic phase. A small heating of the quantum dot will cause the phase transition which results in a jump of the refractive index. Using this technique we are able to increase the photothermal signal by at least a factor of ten. We analyse the photothermal signal in liquid crystals and perform absorption spectroscopy on quantum dots as well as numerical calculations.

CPP 8.13 Mon 17:30 Poster A

**Polymers in an aligned CNT array** — •MARINA KHANEFT<sup>1</sup>, MARKUS DOMSCHKE<sup>1</sup>, BERND STÜHN<sup>1</sup>, RUDOLF FEILE<sup>1</sup>, JÖRG ENGSTLER<sup>2</sup>, and JÖRG SCHNEIDER<sup>2</sup> — <sup>1</sup>Experimentelle Physik kondensierter Materie TU Darmstadt — <sup>2</sup>Eduard Zintl-Institute für Anorganische und Physikalische Chemie TU Darmstadt

An aligned system of carbon nanotubes (CNTs) is obtained by non-catalytic chemical vapor deposition using templates of porous alumina (PAOX) with hexagonally ordered pores and removal of the alumina template. The 3D aligned CNTs array is mechanically stable, flexible and consists of freestanding, parallel aligned CNTs fixed by a car-

bon layer on one side. Obtained CNTs were used for preparation of CNT/polymer composites by melt infiltration of polystyrene (PS) into the free interstices of CNTs structure. Here we present an experimental study of polymer in aligned CNT array. Investigation is focused on the structure of the composites, polymer behaviour near the nanotubes. For quantitative analysis of the structure of the composites and control of the filling process small angle X-ray scattering was used. We applied differential scanning calorimetry to analyse a glass transition of the polymer inside the CNT array depending on the tube diameter and molecular weight of the polymer. Additionally, we applied Brillouin scattering and compare the sound propagation in different CNT/PS composites (vary diameter and molecular weight) with other nanoporous materials filled by polymer. The variation of the Brillouin spectra with the orientation of sample and scattering vector will be discussed.

CPP 8.14 Mon 17:30 Poster A

**Investigation of wetting-dewetting transition of polymer grafted nanoparticles in polymer matrix** — •CHANG JONG KIM<sup>1</sup>, TINKA SPEHR<sup>1</sup>, BERND STÜHN<sup>1</sup>, MARKUS MAZUROWSKI<sup>2</sup>, KATRIN SONDERGELD<sup>2</sup>, ROLAND KLEIN<sup>2</sup>, and MATTHIAS REHAHN<sup>2</sup> — <sup>1</sup>TU Darmstadt, Experimentelle Physik kondensierter Materie — <sup>2</sup>TU Darmstadt, Ernst-Berl-Institut für Technische und Makromolekulare Chemie

The dispersion of nanoparticles in a polymer matrix is generally improved by grafting polymers from the surface of the nanoparticles, when the grafted polymers are miscible with the surrounding matrix. For a given grafting density and molecular weight of grafted polymer the particle dispersion and wetting properties are known to sensitively depend on the ratio of the length of the surrounding polymer matrix to that of the grafted polymer chain. As the length of the matrix polymer chain exceeds that of the grafted polymer, chains of the polymer matrix are dewetted and particles aggregate. In our experiments polystyrene (PS,  $M_n \sim 30\text{kDa}$ ) was grafted from spherical silica (SI) as well as deuterated polystyrene (d-PS) particles. These particles ( $wt \sim 1\%$ ) were dispersed in d-PS matrices with various molecular weights and measured by small angle x-ray scattering (SAXS) and small angle neutron scattering (SANS). The particle dispersion and the change of the conformation (wetting-dewetting transition) of grafted PS chains are probed by analyzing SAXS and SANS scattering curves. First indication for dewetting mechanism were found for PS@d-PS particles when the molecular weight of PS matrix exceeded that of grafted PS.

CPP 8.15 Mon 17:30 Poster A

**Polymerdynamics in Silicabased Nanocomposites with Attractive Interaction** — •BARBARA GOLD<sup>2</sup>, GERALD SCHNEIDER<sup>2</sup>, REINER ZORN<sup>1</sup>, JUERGEN ALLGAIER<sup>1</sup>, WIM PYCKHOUT-HINTZEN<sup>1</sup>, and DIETER RICHTER<sup>1</sup> — <sup>1</sup>Forschungszentrum Jülich GmbH Jülich Centre for Neutron Science (JCNS-1) & Institute of Complex Systems (ICS-1), Forschungszentrum Jülich GmbH, 52425 Jülich — <sup>2</sup>Jülich Centre for Neutron Science (JCNS), Forschungszentrum Jülich GmbH Outstation at FRM II, Lichtenbergstraße 1, 85747 Garching

The interactions between nanoparticles and polymerchains lead to a change in dynamics such as mechanical properties, dielectric relaxation and polymer dynamics.

Also the modification of the parameters within the sample preparation process (amount of solvent, time frame between adding nanoparticles and drying the sample) could modify the actual distribution of the particles as well as these dynamic quantities.

This poster shows the results of SAXS, broadband dielectric and linear rheology measurements concerning a PBO-Silica-System under the variation of particle concentration as well as sample preparation parameters named above.

CPP 8.16 Mon 17:30 Poster A

**Blinking of single CdSe/ZnS nanoparticles on an Al covered silicon substrate** — •ANDREAS MÖLLEKEN, DANIEL BRAAM, GÜNTHER M. PRINZ, MARTIN GELLER, and AXEL LORKE — Fakultät für Physik and CeNIDE, University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany

Semiconductor nanoparticles have attracted great interest as tunable light emitters. They can be easily fabricated without a solid state matrix and therefore placed into different environments and coupled to other nanostructures and metal surfaces. However, a drawback (and a phenomenon that is not yet understood in detail) remains: the blinking and spectral diffusion mechanism in the luminescence behaviour of single nanoparticles [1]. Previous studies have shown that

the blinking behaviour is changed if the nanoparticles are close to a metal surface. In this study, we investigate the coupling between single nanoparticles and an Al metal surface. We fabricate a solution consisting of CdSe/ZnS core/shell nanoparticles dispersed in toluene with 1% PMMA and spin-coat this dispersion on top of an aluminium covered silicon substrate. For the measurements we use a  $\mu$ -PL setup with two different excitation sources (405nm/532nm) in wide-field illumination. The setup enables us to study simultaneously many single nanoparticles and their luminescence behaviour. Our measurements show a blinking behaviour of the emission of single nanoparticles, which we can evaluate in terms of their characteristic on- and off-time statistics. Additionally we observe a slow blue shift in the emission energy over long time periods.

[1] Frantsuzov et al., Nature Phys. 4, 519 (2008)

CPP 8.17 Mon 17:30 Poster A

**DFT studies of clusters in external fields** — •MANUEL MATT, MARCUS BECK, and PETER NIELABA — University of Konstanz, Department of Physics, 78457 Konstanz, Germany

Density functional theory (DFT) studies on the stability and structural properties of small clusters are performed. One point of interest is the arranging of diverse Si nano clusters. We use external electrostatic fields for ordering purposes of these clusters by polarization effects. Here we could stabilize a chain of up to five Si<sub>7</sub> clusters in a Car-Parrinello MD simulation with the CPMD package. We further investigate the Al<sub>13</sub>H cluster which has several isomers with different positions of the hydrogen atom. We analyze the effects of electrostatic and magnetic fields on these systems in order to explore the possibility to switch the isomers by external fields. For this we are using the OCTOPUS package. We found a switching between the two isomers of the neutral Al<sub>13</sub>H cluster at high magnetic fields.

CPP 8.18 Mon 17:30 Poster A

**Separating interface from melt dynamics in a model system** — •CHRISTIAN MARK<sup>1</sup>, MARTIN BRODECK<sup>1</sup>, WIM PYCKHOUT-HINTZEN<sup>1</sup>, JÜRGEN ALLGAIER<sup>1</sup>, EIKE HÜBNER<sup>2</sup>, and DIETER RICHTER<sup>1</sup> — <sup>1</sup>JCNS-1 & ICS-1, Forschungszentrum Jülich GmbH, Jülich, Germany — <sup>2</sup>Institut für Organische Chemie, TU Clausthal, Clausthal, Germany

Designing polymer-based materials with improved properties is an increasingly important field of polymer science. One particular area of interest within that field are the so-called polymer nanocomposites, which are made up of polymer and nanosized filler particles. It is our intent to connect the macroscopic properties of these composite materials to microscopic structure and dynamics.

The dynamics of these systems are, however, a quite difficult topic to study in microscopic detail. This is due to the generally large polydispersity of the nano-components as well as the fact that the measured dynamics are usually a mixture of both interface and melt dynamics. We were able to create grafted nano-sized silica particles ( $r = 7\text{nm}$ ) with a large grafting density (0.7 per square nm, 5K PI), which should provide a sufficient "screen" for separating interface dynamics from melt dynamics. In addition, the grafted particles also allow us to study the dynamics of the grafted polymer chains themselves.

The method used to study the microscopic dynamics is inelastic neutron scattering (Neutron Backscattering and Neutron Spin Echo).

CPP 8.19 Mon 17:30 Poster A

**Synthesis of Semiconductor Nanowires Based on Tubular J-Aggregates Template** — •YAN QIAO, FRANK POLZER, HOLM KIRMSE, EGON STEEG, STEFAN KIRSTEIN, and JÜRGEN P. RABE — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin, Germany

Organic/inorganic hybrid nanomaterials, that combine the strengths of the individual materials while compensating for 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 beneficial influence of dimensionality on electronic and optical properties [1]. Based on former 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 filled with semiconductor nanowires such as ZnO. Owing to electrostatic interactions, zinc ions might adsorb at the outer and inner wall of the negatively charge surface of the tubular J-aggregates. Following the procedures of ammonia precipitation and subsequent heating to moderate temperatures, the transformation from zinc ions into ZnO within the hollow space of the tube

with diameters less than 10 nanometers is supposed to be realized. The as-synthesized inorganic structures are identified by transmission electron microscopy and UV-Vis spectroscopy.

[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 8.20 Mon 17:30 Poster A

**Measuring the range of plasmonic interaction** — MAREIKE KIEL<sup>1</sup>, MADLEN KLÖTZE<sup>1</sup>, STEFFEN MITZSCHERLING<sup>1</sup>, and MATIAS BARGHEER<sup>1,2</sup> — <sup>1</sup>Institute of Physics and Astronomy, University of Potsdam — <sup>2</sup>Helmholtz Zentrum Berlin

When gold nanoparticles are covered with nanometric layers of transparent polyelectrolytes, the plasmon absorption spectrum  $A(\lambda)$  increases by a factor of approximately three and shifts to the red. These modifications of dissipative experimental observables stop when the covering layers become thicker than the particle diameter. The spectral modification of dispersive parameters like the reflection  $R$ , however, keeps changing with increasing cover layer thickness. The shift of the plasmon resonance caused by two interacting particle layers is studied as a function of the separating distance between the two layers. We discuss these observations in the context of an effective medium theory and conclude that it can only be applied for a layer thickness on the order of the particle diameter.

CPP 8.21 Mon 17:30 Poster A

**New Perspectives of Twin-Focus Photothermal Correlation Spectroscopy** — ROMY SCHACHOFF, MARKUS SELMKE, MARCO BRAUN, and FRANK CICHOS — Universität Leipzig, Exp. Phys. I, MONA

Photothermal microscopy has been used successfully for the detection of non-fluorescent nano-objects such as gold nanoparticles, quantum dots or carbon nanotubes. It employs a local temperature field around a laser excited absorber inducing a local refractive index change which is detected by a second laser. A careful investigation of the mechanisms and the origin of the photothermal signal has shown that the photothermal detection volume is in general a twin-focus with two well separated axial detection regions that differ in their signal phase. With the help of this clear spatial separation we are able to measure low axial flow velocities on a short length scale by a cross correlation analysis. We have investigated the diffusion of gold nanoparticles in water by means of this so called Twin-PhoCS. Radiation pressure induced flow velocities are extracted and the detection limits for velocities and small displacements are explored with the help of small gold nanoparticles in the twin-focus.

CPP 8.22 Mon 17:30 Poster A

**Motion and Fluorescence of Charged Single Quantum Dots in an Electric Field** — DAVID PLOTZKI, NICOLE AMECKE, and FRANK CICHOS — Molecular Nanophotonics Group, University Leipzig

Semiconductor Quantum Dots exhibit several interesting optical properties, one of them being a characteristic photoluminescence intermittency (blinking) which is not yet fully understood. It is assumed to be closely linked to charges that influence the underlying relaxation processes.

We study the motion and intensity of CdSe/ZnS Quantum Dots dispersed in toluene and dodecane in the presence of an electric field (up to 200 V/cm). A wide-field microscope setup is used to capture and track the particles. From this, the relative intensities and drift velocities can be determined and conclusions about present charges can be drawn.

We are seeking to observe the exchange of charges at the electrodes by a change in the fluorescence state.

CPP 8.23 Mon 17:30 Poster A

**Scanning transmission x-ray microscopy and quantitative analysis of thermoresponsive microgels** — ANDREAS SPÄTH<sup>1</sup>, BIRGIT GRAF-ZEILER<sup>1</sup>, SHIVKUMAR GHUGARE<sup>2</sup>, GAIO PARADOSSI<sup>2</sup>, and RAINER H. FINK<sup>1</sup> — <sup>1</sup>Friedrich-Alexander Universität Erlangen-Nürnberg, Physical Chemistry II, Erlangen, Germany — <sup>2</sup>Università di Roma Tor Vergata, Scienze e Tecnologie Chimiche, Rome, Italy

Microgels have attracted greater attention in a broad field of medical science. They unify features of macroscopic hydrogels like the connectivity and the responsiveness to environmental changes with the colloidal characteristics of nano- or micro-sized systems. To gain deeper insight into the processes occurring during heating above the volume phase transition temperature, we investigate PVA/poly(methacrylate-co-N-

isopropylacrylamide) based networks using scanning transmission X-ray microspectroscopy. The PoLux-STXM (SLS) combines local-spot chemical information (NEXAFS) and imaging with a resolution limit below 30 nm. Therefore we receive new insight into the nanoscale properties of these materials and directly observe the shrinking behaviour of thermoresponsive microgels in aqueous solution in situ [1]. NEXAFS studies confirm the chemical stability of the particles above the volume phase transition temperature [2]. The qualitative analysis of the received transmittance profiles bases on the Lambert-Beer expression corrected by the finite width of the focused X-ray beam.

[1] Graf-Zeiler, B., et al., *ChemPhysChem*, 2011, DOI: 10.1002/cphc.201100370.

[2] Ghugare, S., et al., *Macromolecules*, 2011, 44 (11), 4470.

CPP 8.24 Mon 17:30 Poster A

**Ellipsometry on GLAD samples: Applications and model calculation** — JOHANNES F. H. RISCH<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>1</sup>, MOTTAKIN M. ABUL KASHEM<sup>1</sup>, GUNTARD BENECKE<sup>1,2</sup>, ADELIN BUFFET<sup>1</sup>, DENISE ERB<sup>1</sup>, BERIT HEIDMANN<sup>1</sup>, GERT HERZOG<sup>1</sup>, VOLKER KÖRSTGENS<sup>3</sup>, EZZELDIN METWALLI<sup>3</sup>, ROMAN MANNWEILER<sup>1</sup>, JAN PERLICH<sup>1</sup>, ANDRÉ ROTHKIRCH<sup>1</sup>, KAI SCHLAGE<sup>1</sup>, PETER MÜLLER-BUSCHBAUM<sup>3</sup>, RALF RÖHLSBERGER<sup>1</sup>, RAINER GEHRKE<sup>1</sup>, and STEPHAN V. ROTH<sup>1</sup> — <sup>1</sup>DESY, Notkestr. 85, D-22607 Hamburg — <sup>2</sup>MPIKG, Dep. Biomat, Am Mühlenberg 1, D-14424 Potsdam-Golm — <sup>3</sup>TU München, Physik Department E13, James-Frank-Str. 1, D-85748 Garching

Polymers combined with metals have a wide field of application in technology and industry. For the installation of tunable optical properties in nanocomposites, glancing angle deposition (GLAD) [1] has been proven to be a reliable method due to the high acceptance of vacuum sputter deposition in industrial processes. We investigated glancing angle deposition of gold on top of a colloidal array (polystyrene nanospheres), which serves as nucleation points for gold clusters. Using Imaging ellipsometry, we investigated the change of optical properties caused by structural deposition of polystyrene-nanospheres and gold layers. On the basis of gold pins, being inclined with respect to the surface normal, on polystyrene spheres we obtain a change of the refraction indices and a varying apparent layer thickness as function of the orientation of the GLAD sample.

[1] Gonzalez-Garcia et al., *ChemPhysChem* 11, 2005 (2010)

CPP 8.25 Mon 17:30 Poster A

**Humidity-tunable electronic conductivity of polyelectrolyte multilayers doped with Au-nanoparticles** — ANNIKA ZIEGEMEIER, CORNELIA CRAMER, and MONIKA SCHÖNHOF — Institute of Physical Chemistry, Westfälische Wilhelms-Universität Münster, Corrensstr. 28/30, 48149 Münster, Germany

The dc conductivity of polyelectrolyte multilayers doped with gold nanoparticles (Au-nP) was investigated as a function of relative humidity. For this purpose, multilayers composed of poly(ethyleneimine) (PEI) or poly(allylamine hydrochloride) (PAH) and Au-nP (diameter about 20 nm) were built up using the layer-by-layer self assembly technique. Different polyelectrolytes and varying salt concentrations lead to differences in the total layer thickness and the Au-nP coverage, i.e. different interparticle distances. The dc conductivity of the doped systems is six orders of magnitude higher than that of ions in undoped multilayers, thus an electronic conductivity can be concluded. Electrons are transported via connected pathways of Au-nP, as concluded from the conductivity scaling inversely with the expected particle distance in different systems. With increasing relative humidity (RH) the dc conductivity decreases and reversibly increases again when RH is decreased. It is concluded that the swelling of the polyelectrolyte chains between adjacent particles leads to a loss of connectivity of the electronic pathways between single particles, driving the system closer to the percolation threshold, and resulting in a decrease of conductivity. In conclusion, the conductivity of polyelectrolyte multilayers doped with Au-nP can be reversibly tuned by varying the relative humidity.

CPP 8.26 Mon 17:30 Poster A

**Studies on microgel-polymer blends** — FLORIAN SCHNEIDER<sup>1</sup>, GERALD JOHANNES SCHNEIDER<sup>1</sup>, ANDREEA BALACEANU<sup>2</sup>, ANDRIJ PICH<sup>2</sup>, WIM PYKHOUT-HINTZEN<sup>3</sup>, JÜRGEN ALLGAIER<sup>3</sup>, and DIETER RICHTER<sup>3</sup> — <sup>1</sup>Jülich Centre for Neutron Science, 85747 Garching, Germany — <sup>2</sup>DWI an der RWTH Aachen e.V., 52056 Aachen, Germany — <sup>3</sup>Jülich Centre for Neutron Science & Institute for Complex Systems, Forschungszentrum Jülich GmbH, 52425 Jülich

Microgels are formed by crosslinking of single polymer chains. Possible characteristics of the resulting structures can include sensitivity to light, temperature and to chemical properties of the solvent. The response of the gel affect it's physical structure, for example changes in particle size or density. Up to now, studies mainly concentrate on microgels dissolved in water.

Combining the idea of filler particles to tune the properties of a polymer matrix with the concept of microgels, new and interesting composites can be imagined. Not only does the usage of soft, organic fillers result in lower compound weights, it also opens the possibility to influence the composites' properties by varying external parameters.

Our studies are based on custom poly(vinylcaprolactam) microgels. Their physical structure and it's dependence on the properties of the solvent as well as the possibility of dispersing them in a polymer matrix were resolved by different neutron scattering techniques. Moreover first results concerning their influence on the dynamics of a polymer matrix were obtained in rheology-experiments.

CPP 8.27 Mon 17:30 Poster A

**Surface Charges on CdSe/ZnS Quantum Dots in Apolar Solvents** — •NICOLE AMECKE and FRANK CICHOS — Molecular Nanophotonics Group, University of Leipzig

Despite intensive research, semiconductor quantum dots (QDs) show many peculiar fluorescence characteristics (blinking, flickering, spectral diffusion) that are not fully understood today. Many of those are expected to be strongly influenced by charges in the QD core or its close proximity. With a confocal microscope and an electrophoretic cell, charged QDs in solution can be detected and separated from neutral QDs while monitoring their fluorescence. Depending on solvent and electrode characteristics we find the percentage and polarity of detected fluorescent charges to differ, showing a manipulation of the charges at the electrode. This charging of QDs and their total percentage can also be detected by the current flowing through the device. Spectra and lifetimes from charged and neutral QDs are taken separately and compared. As only minor differences are found, the charge must be located at the surface not in the core.

CPP 8.28 Mon 17:30 Poster A

**Polymer-Functionalized Carbon Structures: A Raman Spectroscopy View** — •EVGENIYA SHEREMET, RAUL D. RODRIGUEZ, THOMAS EBERT, SUSANNE HÖHNE, STEFAN SPANGE, OVIDIU D. GORDAN, and DIETRICH R. T. ZAHN — Chemnitz University of Technology, D-09107 Chemnitz, Germany

Raman spectroscopy is a powerful technique for structural studies of polymer-coated carbon structures. Here, we discuss the challenges of obtaining reliable Raman data and their interpretation using several model systems: phenolic resin on graphite flakes and poly(ethylhexylacrylate) with a pyrene headgroup, polyvinylamin, and polyacrylamide adsorbed on multi-wall carbon nanotubes (MWCNT). It is shown that such composites reveal clear G and D bands (around  $1582\text{ cm}^{-1}$  and  $1350\text{ cm}^{-1}$ , respectively) characteristic of carbon structures with  $sp^2$  hybridization, and modifications induced by the polymer coating are discussed. From all polymers studied the largest degree of interaction with MWCNT was found for poly(ethylhexylacrylate) as deduced from an upward shift of the G peak mostly likely due to compressive forces induced by the polymer on the nanotube walls. However, organic materials, as well as carbon structures, can be strongly affected by laser irradiation. It was shown that phenolic resin is removed by UV excitation, what resulted in a decrease in its Raman signature. Pure MWCNT also demonstrate a decrease of D peak after laser irradiation. In this work a systematic analysis of D and G band shifts in Raman spectroscopy of polymer-carbon composites is presented.

CPP 8.29 Mon 17:30 Poster A

**Particle Nanosomes with Tailored Silhouettes** — CLAUDIA WAGNER<sup>1</sup>, •ANDREA FORTINI<sup>2</sup>, EDDIE HOFMANN<sup>1</sup>, THOMAS LUNKENBEIN<sup>3</sup>, MATTHIAS SCHMIDT<sup>2</sup>, and ALEXANDER WITTEMANN<sup>1</sup> — <sup>1</sup>Physikalische Chemie I, Universität Bayreuth, Universitätsstr. 30, D- 95440 Bayreuth, Germany — <sup>2</sup>Theoretische Physik II, Universität Bayreuth, Universitätsstr. 30, D-95440 Bayreuth, Germany. — <sup>3</sup>Anorganische Chemie I, Universität Bayreuth, Universitätsstr. 30, D- 95440 Bayreuth, Germany.

We investigate the assembly of submicron capsules with walls that consist of a single layer of nanoscopic inorganic constituents. Nanoparticles and oppositely charged polymer colloids were joined at the surface of evaporating emulsion droplets. The heteroaggregates exhibited

well-defined core-shell morphologies, with clusters of the polymer colloids as the core and a dense monolayer of nanoparticles as the shell. Subsequent removal of the polymer core led to capsules, which exhibited regular compartmentalized shapes. A high density of nanopores was obtained on objects with dimensions of less than half a micron. Regardless that the capsules consisted of a single layer of nanoparticles with few contacts keeping them together, they did not collapse or break apart. Monte Carlo computer simulations demonstrated that the nanoscopic constituents can be trapped into structurally arrested states.

CPP 8.30 Mon 17:30 Poster A

**Preparation and Controlled Organization of Cubic-Shaped Gold Nanoparticles for the Generation of High-Harmonics** — •VALERIE MONDES<sup>1</sup>, SARAH METZKE<sup>1</sup>, MATTHIAS BUCHHOLZ<sup>1</sup>, MATTHIAS KLING<sup>2</sup>, JÜRGEN PLENKE<sup>1</sup>, ECKART RÜHL<sup>1</sup>, and CHRISTINA GRAF<sup>1</sup> — <sup>1</sup>Freie Universität Berlin, Institut für Chemie und Biochemie, Physikalische und Theoretische Chemie, Takustr. 3, 14195 Berlin — <sup>2</sup>Max-Planck Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching

Strong plasmonic enhancement effects are expected from ordered patterns of anisotropic noble metal nanoparticles. Instead of using lithographically fabricated nanostructures, we prepare gold nanoparticles by methods of colloidal chemistry. For the preparation of cubically shaped gold nanoparticles we improved known literature procedures [1]. The conditions during the formation of the nanoparticles have been systematically varied in order to receive monodisperse gold nanocubes. It turned out that the exact composition of the shape-controlling surfactant cetyltrimethylammonium bromide (CTAB) plays a crucial role for the growth of the nanoparticles. Therefore, CTAB samples were purchased from different manufactures and their composition was analyzed regarding the presence of other halides, which are supposed to influence the particle growth. In addition, the influence of the temperature has been investigated. A self-organization method at liquid-liquid interfaces has been used to receive such ordered particle assemblies [2]. [1] P.N.Sisco, C.J.Murphy, J.Phys.Chem. A, 113, 3973 (2009). [2] Li, Huang, and Sun Angew. Chem. Int. Ed., 45, 2537 (2006).

CPP 8.31 Mon 17:30 Poster A

**Photoluminescence quantum yield of near-infrared emissive nanoparticles** — •SOHEIL HATAMI<sup>1</sup>, CHRISTIAN WÜRTH<sup>1</sup>, MARKUS GRABOLLE<sup>1</sup>, SUSANNE LEUBNER<sup>2</sup>, VLADIMIR LESNYAK<sup>2</sup>, NIKOLAI GAPONIK<sup>2</sup>, ALEXANDER EYCHMÜLLER<sup>2</sup>, and UTE RESCH-GENGER<sup>1</sup> — <sup>1</sup>BAM Federal Institute for Materials Research and Testing, Berlin, Germany — <sup>2</sup>Physical Chemistry/Electrochemistry, TU Dresden, Dresden, Germany

Semiconductor nanocrystals (quantum dots, QDs) are applied as fluorescent labels and active components in optical devices. QDs emitting in the near-infrared (NIR) and infrared (IR) region like CdTe, CdHgTe, and HgTe are of increasing importance, due to their high photoluminescence quantum yields (QY) compared to any other chromophore at wavelengths above 900 nm. Characterization of their performance requires reliable methods for the determination of QY under application-relevant conditions. For often performed relative optical measurements, standard dyes with precisely known QY are mandatory, with the lack of reliably assessed QY standards for the NIR and IR hampering the performance of such measurements. We established relative and absolute optical methods for the determination of QY of such QDs in this wavelength region. Therewith, we obtained the QY of these QDs from 1.) comparison of the integral emission of the QDs and standard dyes and 2.) absolute measurements of the ratio of emitted and absorbed photons using a calibrated and validated integrating sphere setup.

CPP 8.32 Mon 17:30 Poster A

**Probing the electronic state of a single coronene molecule by the emission from proximate fluorophores** — •KATHRIN SCHNEIDER<sup>1</sup>, BURKHARD FÜCKEL<sup>1</sup>, GERALD HINZE<sup>1</sup>, KLAUS MÜLLEN<sup>2</sup>, and THOMAS BASCHE<sup>1</sup> — <sup>1</sup>Institut für Physikalische Chemie, Johannes Gutenberg-Universität, 55099 Mainz — <sup>2</sup>Max-Planck-Institut für Polymerforschung, 55128 Mainz

Electronic transitions of the 2D-graphene type molecule hexabenzocoronene (HBC) have been measured at the single molecule level. The large intersystem crossing rate and long triplet state lifetime in the range of seconds are prohibitive for direct single molecule observation. By covalently coupling fluorescent acceptor molecules (perylene-carboximide, PMI) to HBC, efficient singlet energy transfer gives rise

to strong PMI fluorescence. Confocal single molecule fluorescence microscopy with two excitation colours matching the HBC and PMI transition frequencies, respectively, was conducted. Single HBC-6PMI molecules were observed via the PMI emission. It was found that after selective excitation of the HBC the PMI emission is interrupted by dark intervals whose length of several seconds is in agreement with the triplet state lifetime of HBC. Accordingly, the presence/absence of PMI emission permits to read out the spin state of a single HBC molecule. Moreover, due to spectral overlap, the HBC triplet state acts as an energy acceptor for PMI in the excited singlet state, thus leading to efficient singlet-triplet annihilation (STA) during its lifetime. Hence, intersystem crossing into the HBC triplet state serves as a collective fluorescence switch for individual multichromophores.

CPP 8.33 Mon 17:30 Poster A

**Investigation of interphases in poly(ethylene-propylene)(PEP)-silsesquioxane-nanocomposites by positron annihilation lifetime spectroscopy** — •CHRISTIAN OHRT<sup>1</sup>, TÖNJES KOSCHINE<sup>1</sup>, STEPHAN HARMS<sup>1</sup>, KLAUS RÄTZKE<sup>1</sup>, FRANZ FAUPEL<sup>1</sup>, GERALD SCHNEIDER<sup>2</sup>, LUTZ WILLNER<sup>2</sup>, and DIETER RICHTER<sup>2</sup> — <sup>1</sup>Materialwissenschaft-Materialverbunde, Universität Kiel, 24143 Kiel — <sup>2</sup>Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich

Free volume studies were performed in polymer-nanocomposites by positron annihilation lifetime spectroscopy (PALS) to explore the influence of the interphase nanoscale character of the filler particles and the nanoscale particle size on positron parameters. A weakly repulsive system was obtained by mixing of poly(ethylene-alt-propylene) (PEP) and silsesquioxane nanoparticles with varying concentration. DSC experiments showed a constant glass transition temperature  $T_g$  of the polymer and a phase transition of the filler at low temperature. PALS measurements showed a constant glass transition temperature  $T_g$  of the polymer, an increase of the free volume at the phase transition of the filler and a strong drop of the thermal expansion coefficient above  $T_g$  with increasing filler concentration. By changing the composition of the samples and applying a simple mixing rule for the lifetime spectra of the ortho-positronium, information about the existence of an interphase with properties different from the polymer matrix could be obtained.

CPP 8.34 Mon 17:30 Poster A

**Evolution of lateral structures during the functional stack build-up of P3HT:PCBM based bulk heterojunction solar cells** — •SHUAI GUO<sup>1</sup>, MATTHIAS RUDERER<sup>1</sup>, CHRISTOPHER BIRKENSTOCK<sup>1</sup>, EZZELDIN METWALLI<sup>1</sup>, MONIKA RAWOLLE<sup>1</sup>, JAN PERLICH<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany — <sup>2</sup>HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

Solution-processable organic photovoltaics have shown great promise for providing an entirely new generation of ultralow-cost, lightweight, and flexible electronic devices, which would be an ideal alternative to replace the traditional expensive silicon-based semiconductors. Here, the most prominent material system 1,2-dichlorobenzene solution processed P3HT:PCBM bulk heterojunction (BHJ) solar cells, are prepared and investigated at different steps of the multi-layer stack build-up. The inner structural characteristics are probed with grazing incidence small angle X-ray scattering (GISAXS) and X-ray reflectivity. The surface morphology is detected with atomic force microscopy. Therefore, an in-depth knowledge of three-dimensional morphology of the polymer-based solar cell, starting from the cleaned ITO substrate up to the final post-treated solar cell, is generated. Three noticeable lateral structures, originating from the substrate, the active layer and the aluminum electrode, are detected with GISAXS. The correlation between nanostructure within the thin films and the solar cell efficiency are addressed.

CPP 8.35 Mon 17:30 Poster A

**Structure-property relationship of Nanocomposites based on Polylactide and Layered Double Hydroxide** — •PURV PUROHIT and ANDREAS SCHÖNHALS — BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany

Nanocomposites based on biopolymer Polylactide (PLA) and organically modified MgAl Layered Double Hydroxide (MgAl-LDH) were prepared and investigated by a combination of differential scanning calorimetry (DSC), Small and Wide angle X-ray scattering (SAXS & WAXS) and Dielectric Relaxation Spectroscopy (DRS). DSC and WAXS show that the degree of crystallinity is influenced by the con-

tent of LDH. The dielectric response of the nanocomposites shows several relaxation processes. The intensity of the dynamic glass transition increases with the concentration of LDH. This is attributed to the increasing concentration of the exchanged anion sodium dodecylbenzene sulfonate (SDBS), which are adsorbed at the LDH layers. Two processes are identified at lower and higher temperatures both having a signature of the dynamic glass transition. The process at lower temperature originates from polymer segments close to the LDH whereas the one at higher temperature (bulk like) from the molecules at a farther distance from the LDH. Other than these two processes,  $\beta$  relaxation is identified which is related to localized fluctuations in the polymer chain.

CPP 8.36 Mon 17:30 Poster A

**Electrical investigation of gold nanoparticles using heterojunctions based on strained nanomembranes** — •MARIA BENDOVA<sup>1</sup>, CARLOS CESAR BOF BUFON<sup>1</sup>, SANDEEP GORANTLA<sup>2</sup>, MARK H. RÜMMELI<sup>2</sup>, and OLIVER G. SCHMIDT<sup>1</sup> — <sup>1</sup>Institute for Integrative Nanosciences, IFW Dresden, Germany — <sup>2</sup>Institute for Solid State Research, IFW Dresden, Germany

In this work we present the investigation of electrical transport across mono-/bilayers of capped Au nanoparticles (NPs) vertically contacted using strained nanomembranes [1]. The fabrication process consists of a strained Au nanomembrane which rolls up on top of a metal finger structure where the NPs layer was previously deposited. The strained nanomembrane-based electrode provides a soft yet robust contact on top of NPs. The fabrication process is compatible with standard micro-fabrication techniques and several devices can be created in parallel on a chip. This represents an advantage when compared with other contacting methods (STM, nanogap electrodes).

The transport measurements exhibit Coulomb blockade and Coulomb staircase behavior at 4 K, which is correlated with NPs size and the presence of organic tunneling barriers. The Coulomb peaks in the differential conductance spectra vanish above 50-70 K as the thermal energy exceeds the NPs charging energy. Thus, this method can be directly employed to contact various types of nanoparticulate materials, whereas averaged properties of a macroscopic set of NPs (areas of  $\mu\text{m}^2$ ) can be obtained.

[1] C. C. B. Bufon et al., *Nano Lett.*, **2011**, 11, 3727.

CPP 8.37 Mon 17:30 Poster A

**Förster resonance energy transfer (FRET) experiments on tubular J-aggregates wrapped with dye labeled polyelectrolytes** — •OMAR AL-KHATIB<sup>1</sup>, CHRISTOPH BÖTTCHER<sup>2</sup>, HANS VON BERLEPSCH<sup>2</sup>, JÜRGEN P. RABE<sup>1</sup>, and STEFAN KIRSTEIN<sup>1</sup> — <sup>1</sup>HU Berlin, Inst. für Physik Newtonstr. 15, 12489 Berlin — <sup>2</sup>FU Berlin, Forschungszentrum für Elektronenmikroskopie, Fabeckstr. 36a, 14195 Berlin

In this contribution we demonstrate the coating of tubular J-aggregates with dye-labeled polyelectrolytes. The tubular J-aggregates are formed by an amphiphilic cyanine dye in aqueous solutions [1]. These aggregates can be considered as cylindrical objects with 13 nm diameter, length exceeding microns and a negative surface potential. It is shown by cryogenic electron microscopy (cryo-TEM) that polycations can be adsorbed at the aggregate surface forming a homogeneous coating layer. Poly(diallyldimethyl ammonium chloride) (PDAC) and poly(allylamine hydrochloride) (PAH) labelled with different fluorescent dyes are used, acting as donors or acceptors within a Förster energy transfer (FRET) process. The donor and acceptor dyes are distributed homogeneously within the coating. The FRET is investigated by static optical absorption and fluorescence spectroscopy. The experiments demonstrate the possibility for symmetric energy transfer from donors to the aggregate and from the aggregate to acceptors. No indication for enhanced energy transfer due to exciton diffusion was found. [1] D.M. Eisele, et al., *Nature Nanotech.* **4** (2009) 658;

CPP 8.38 Mon 17:30 Poster A

**In-situ sputter deposition: from early stages to final layer growth as seen by in-situ GISAXS** — •STEPHAN V. ROTH<sup>1</sup>, RALPH DOEHRMANN<sup>1</sup>, Gerd HERZOG<sup>1</sup>, GUNTARD BENECKE<sup>1,2</sup>, STEPHAN BOTTA<sup>1</sup>, ADELINE BUFFET<sup>1</sup>, BERIT HEIDMANN<sup>1</sup>, RAINER GEHRKE<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>1,3</sup>, EZZELDIN METWALLI<sup>4</sup>, and PETER MUELLER-BUSCHBAUM<sup>4</sup> — <sup>1</sup>DESY, Notkestr. 85, D-22607 Hamburg — <sup>2</sup>MPIKG, Dep. Biomater., Am Mühlenberg 1, D-14424 Potsdam-Golm — <sup>3</sup>Univ. Hamburg, Inst. Techn. Makromol. Chem., Bundesstr. 45, D- 20146 Hamburg — <sup>4</sup>TU München, Physik Department, LS Funkt. Mat., James-Frank-Str. 1, D-85748 Garching

Understanding the growth kinetics of metal polymer nanocomposites is of utmost importance to tailor the structure-function relationship for materials in modern technologies [1]. The key point during the processing of these nanocomposites is the interaction between the metal atoms and the underlying polymer layer(s) [2,3]. As sputter deposition is one of the most widely used industrial methods for rapid metal coating, we investigate the gold layer growth on top of a thin, spin-coated polystyrene film in-situ using microbeam grazing incidence small-angle x-ray scattering ( $\mu$ GISAXS) with high temporal resolution. We follow the different stages of nanoparticle formation from the initial correlated roughness changes induced by deposition to the fully established layer. We present the full morphological and structural characterization as function of deposition time and gold layer thickness.

[1] Faupel et al., Adv. Eng. Mat. 12, 1177 (2010); [2] Metwalli et al., Langmuir 24, 4265 (2008); [3] Buffet et al., Langmuir 27, 343 (2011)

CPP 8.39 Mon 17:30 Poster A

**Density Matrix Description of Molecule Metal Nanoparticle Interactions** — •GEROLD KYAS, YAROSLAV ZELINSKY, YUAN ZHANG, and VOLKHARD MAY — Institut für Physik, Humboldt-Universität zu Berlin, Germany

Within the emerging field of plasmonics, particular efforts are undertaken to gain a fundamental insight into the interaction between molecules and metal nanoparticles (MNPs). Recent experimental and theoretical studies demonstrated a versatile enhancement effect of the metal supporting various molecular processes, such as light absorption, emission and intermolecular charge and energy transfer. In our approach, we describe these phenomena via a density matrix based microscopic theory, which, in contrast to the proposals made in other works, is fully quantum mechanical and hence free of the need to calculate local electric fields.

As an application, we present a consideration of MNP affected intermolecular excitation energy transfer [1]. Moreover, the emission and absorption spectra of molecular complexes placed in close vicinity to an MNP are discussed [2]. Finally, we briefly comment on plasmon assisted charge transmission through a molecular junction.

[1] G. Kyas and V. May, J. Chem. Phys. 134, 034701 (2011).  
[2] Ya. R. Zelinsky and V. May, Chem. Phys. Lett. 511, 372 (2011).

CPP 8.40 Mon 17:30 Poster A

**Modified Guest Chains in Dense Polymer Brushes** — •DIRK ROMEIS<sup>1,2</sup>, HOLGER MERLITZ<sup>1,3</sup>, and JENS-UWE SOMMER<sup>1,2</sup> — <sup>1</sup>Leibnitz-Institut für Polymerforschung e.V., 01069 Dresden — <sup>2</sup>TU Dresden, Fachbereich Physik, 01062 Dresden — <sup>3</sup>Department of Physics and ITPA, Xiamen University, Xiamen 361005, P. R. China

Using a quasi off-lattice self-consistent field approach we systematically study the behavior of modified guest chains in densely grafted polymer brushes. The presented approach accounts for finite extensible chains of spherically shaped monomers and the Carnahan-Starling equation of state for hard spheres is applied. Recent MD simulations [1] found significant conformational instabilities for the guest chains, which could be reproduced in quantitative agreement. A simple analytical model is developed, which confirms the encountered scaling laws for the observed conformational transition.

[1] Merlitz H. et. al. [*Macromolecules* 41 5070, 2008].

CPP 8.41 Mon 17:30 Poster A

**Photo-fluorescence spectroscopy of a novel form of ultra-stable silicon nanoparticles** — HANIEH YAZDANFAR, GEDIMINAS GALINIS, GAUTHIER TORRICELLI, MARK WATKINS, ATEA AKRAIAM, and •KLAUS VON HAEFTEN — Department of Physics and Astronomy, University of Leicester, Leicester, LE1 7RH, United Kingdom

Silicon nanoparticles produced by a novel co-deposition technique [1] show a number of extraordinary properties: clusters smaller than 3 nm in diameter form a stable phase in water, do not agglomerate [2] and emit strong and exceptionally stable fluorescence when excited with UV light [3]. An unequivocal assignment of the fluorescence is challenging because of the breadth of possible geometric structures and cluster sizes. We found the fluorescence wavelength un-shifted irrespective of the excitation energy and concluded that the fluorescent transitions originated from localised defects presumably caused by a chemical reaction of silicon with water. In alcoholic solvents the clusters fluoresce as well but the bands exhibit a blue-shift which we found to correlate with the dipole moment of the solvent molecules and which we interpreted as evidence for a location of the defects at the cluster

surface. Size effects were investigated by AFM of clusters placed on HOPG in UHV and by filtering the solutions, which revealed that the fluorescence stemmed only from the smaller clusters in the solution.

[1] K. von Haeften et al. Eur. Phys. J. D 52, 11 (2009).  
[2] A. Brewer, K. von Haeften, Appl. Phys. Lett. 94, 261102 (2009).  
[3] G. Torricelli, A. Akraiam, K. von Haeften, Nanotechnology 22, 315711 (2011).

CPP 8.42 Mon 17:30 Poster A

**Tailoring the blinking behaviour of single CdSe/ZnS nanoparticles** — •DANIEL BRAAM, ANDREAS MÖLLEKEN, GÜNTHER M. PRINZ, MARTIN GELLER, and AXEL LORKE — Fakultät für Physik and CeNIDE, University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany

Though CdSe/ZnS nanoparticles have been investigated over the last decades, their emissive behaviour still lacks a complete understanding. Single particle photoluminescence (PL) measurements have the ability to give insight into the underlying recombination processes. With a custom-built  $\mu$ -PL setup, using a LN<sub>2</sub> cooled CCD-camera attached to an imaging spectrometer, we can acquire time-resolved 2D-images of several nanoparticles to investigate them and their blinking statistics simultaneously. Specific particles can be selected for further spectral characterisation. Here, we focus on the influence of different rough metal layers on the brightness and stability of the luminescence. We observe intensity enhancement, which we attribute to plasmonic effects, and continuous blue shifts of several tens of nanometers during illumination, which is accompanied by randomly varying stark shifts. At low temperatures ( $\leq 10$  K) some particles show spectral jumps of 25 meV instead of blinking, which indicate altered radiative and non-radiative recombination rates induced by the aluminium layer.

CPP 8.43 Mon 17:30 Poster A

**Functionalized Luminescent Silicon Quantum Dots** — •MARC WEGMANN, GEORG BREHM, and CAROLA KRYSCHI — Friedrich-Alexander University of Erlangen, Egerlandstr. 3, 91058 Erlangen, Germany

One of the central challenges in fabrication of luminescent Si quantum dots (SiQDs) tailored for nano-optoelectronics is to functionalize their surfaces with electronically efficiently coupled molecules that mediate carrier injection into the bulk and allow to optically control charge separation as well as luminescence properties of the bulk. In this contribution we will present a detailed spectroscopy study of bright green-luminescent alkenyl-passivated SiQDs with were prepared via a four-step wet-chemistry synthesis route. The sizes, crystallinity and shapes as well as the surface structures of differently functionalized SiQDs were examined employing high-resolution transmission electron microscopy (HRTEM) and FTIR spectroscopy, respectively. Stationary and time-resolved photoluminescence spectroscopy experiments provided essential information of luminescent surface and bulk states. The interplay between electronically excited molecular states and conduction band states was examined upon directly monitoring photo-excited carrier dynamics with femtosecond transient absorption and luminescence up conversion spectroscopy.

CPP 8.44 Mon 17:30 Poster A

**Concave Micro/Nanoparticles as Powerful Facilitators for Bonding of Non-Adhesive Polymers** — •XIN JIN<sup>1</sup>, SEBASTIAN WILLE<sup>1</sup>, DAWIT GEDAMU<sup>1</sup>, RAINER ADELUNG<sup>1</sup>, JAN STRÜBEN<sup>2</sup>, ANNE STAUBITZ<sup>2</sup>, LARS HEEPE<sup>3</sup>, ALEXANDER KOVALEV<sup>3</sup>, and STANISLAV GORB<sup>3</sup> — <sup>1</sup>Functional Nanomaterials, Institute for Materials Science, University of Kiel — <sup>2</sup>Otto-Diels Institute of Organic Chemistry, University of Kiel — <sup>3</sup>Functional Morphology and Biomechanics, Institute of Zoology, University of Kiel

Modern engineering often requires that two polymer objects are firmly joined together, while at the same time demanding that specific properties and functions of each individual polymer are preserved. In many cases, chemical and mechanical properties of polymers to be joined are so different that strong adhesive bond between them by using conventional methods is hardly possible. In this work, we present a new approach to facilitate strong adhesion between non-adhesive polymers, such as PTFE and crosslinked PDMS, by employing tetrapod ZnO micro/nanoparticles with concave cross-section. We show that the adhesion force attained by this approach is of the same order of magnitude as obtained by plasma etching method and can be seen as a viable, simple alternative to this method. The tetrapod micro/nanoparticles were produced in high quantities at low cost with Flame Transport Synthesis (FTS). Results from peeling tests, SEM observations, and



video recordings of peeling process are presented. The mechanisms of adhesion enhancement are discussed in detail. Acknowledgement: We thank DFG SFB677-C10 for the financial support.

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**Transmission electron microscopy investigation of a gold / TiO<sub>2</sub> catalyst** — ●KRISTIAN FRANK, ANDRE WICHMANN, ARNE WITTSTOCK, LUTZ MÄDLER, MARCUS BÄUMER, and ANDREAS ROSENAUER — Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

Nanoporous gold is a material for many applications e.g. in catalysts, sensors and electrode materials. It is created by chemical etching of a gold - silver alloy. Important structural properties are the pore size and the size of the gold ligaments. For the application in catalysis of CO-oxidation, the gold can be coated with TiO<sub>2</sub> in order to enhance catalytic activity. In the temperature range above 60 °C the CO conversion of the TiO<sub>2</sub> coated sample is increased by more than one order of magnitude compared with the pure nanoporous gold. The structure and distribution of the TiO<sub>2</sub> on the gold surface is an important property, which was investigated by TEM. It was shown, that the gold ligaments are abundantly covered by approximately 5 nm TiO<sub>2</sub> particles. The determination of the largest lattice fringe distance with HR-TEM revealed that the crystalline nanoparticles consist of the anatase phase. The spatial Ti distribution was measured with EFTEM (energy filtered TEM).

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**The ordering of dodecyl chains and their influence on the agglomeration of zirconia nanoparticles** — ●SILVIA PABISCH<sup>1</sup>, BERNHARD FEICHTENSCHLAGER<sup>2</sup>, GUIDO KICKELBICK<sup>3</sup>, and HERWIG PETERLIK<sup>1</sup> — <sup>1</sup>University of Vienna, Faculty of Physics, Vienna, Austria — <sup>2</sup>Vienna University of Technology, Institute for Materials Chemistry, Vienna, Austria — <sup>3</sup>Saarland University, Inorganic Solid State Chemistry, Saarbrücken, Germany

The ordering of dodecyl chains has been investigated in mixed monolayers of phosphonic acid capping agents on the surface of hydrothermal prepared zirconia nanocrystals. As co-capping agent for the mixed monolayer formation, methyl-, phenyl-, pyryl- and tert-butyl phosphonic acid have been used to investigate series with different mixing ratios with dodecyl phosphonic acid. In this study, the influence of the various molecules on the alkyl chain disordering is discussed. Small angle X-ray scattering (SAXS) studies show that with increasing amount of co-capping agent the agglomeration of the particles decreases. This behavior correlates with the ordering of the surface bond alkyl chains investigated by Fourier transform infrared spectroscopy (FTIR). It can be concluded that interparticle bilayers, formed via long alkyl chain packing, are responsible for the formation of dense particle agglomerates and can be controlled on a molecular level by co-adsorbing various molecules. Based on this correlation nanoparticles can be used as probes for self-assembled monolayer investigation by an indirect method (SAXS) and correlated with the routine method for the chemical analysis of surface groups (FTIR).

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**AFM investigations of surface properties of 2, 4, 6 trinitrophenol (TNP) crystal at the nanoscale** — ●ALEXANDER KOVALEV<sup>1</sup> and HEINZ STURM<sup>1,2</sup> — <sup>1</sup>BAM - Fed. Inst. Materials Res. - Div. Nanotribology and Nanostructuring, 12205 Berlin — <sup>2</sup>TU Berlin, IWF, 10587 Berlin

Knowledge of the behaviour of energetic materials (EM) subjected to phenomena at the nanometre scale is a main key to better understanding the nature of initiation processes of an explosion. The chemical-mechanical decomposition of EM is not fully understood, and the initial decomposition steps are not firmly established, but the model of hotspot formation is generally accepted. The initial size of a hotspot is comparable with molecular dimensions of EM. It is evident that the real origin of ignition should be explored at the nanometre scale, and such possibility are provided by atomic-force microscopy (AFM) techniques. Here, we report on the direct initiation of the hotspot formation on surfaces of 2, 4, 6-trinitrophenol (TNP) single crystals by the AFM tip. The immediate AFM imaging of the selected region revealed the destructive changes of TNP crystals, and allows a first estimate of the evolution of hotspot phenomenon at the initial stage. The direct observation of the nanoscale surface restructuring of TNP crystal during the AFM scanning has been explored. Our results reveal the instability of TNP molecules at the border of molecular layers at normal ambient condition. Based on the explored properties of TNP

crystal a mechanism of hotspot formation at the nanoscale is proposed.

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**Probing nanomechanical structure-property relationships of micro- and nanofibers by AFM bending experiments** — DANIEL KLUGE and ●ANDREAS FERY — Physikalische Chemie II, Universität Bayreuth, Universitätsstraße 30, 95440 Bayreuth, Germany

Micro- and nanofibers are important structural elements in biomaterials and tissues, where one of their main functions is providing mechanical stability. Characterizing these small-scale fibers requires highly specialized techniques beyond standard methods for macroscopic materials. Nanoscale bending of the fibers is a common approach and applicable for a wide variety of fiber systems.

In our contribution, we focus on bending experiments of fibers suspended over channels: We show results on bending perpendicular and parallel to the substrate plane. We will discuss major advantages of these two bending modes, for example validation of boundary conditions, direct integration of optical methods and detailed investigation of the mechanical properties beyond linear elastic deformations.

Our experiments allow us to investigate the properties of numerous novel materials and we will present in detail our studies on supramolecular benzenetrisamide aggregates. Small changes in their molecular structure can significantly influence their morphology, which makes them suitable for "bottom-up" tailored materials. We look into the effect of the molecular structure on their mechanical behavior and compare benzenetrisamide whiskers and fibers obtained by different preparation methods.

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**Nuclear Quantum Effects of Liquid Water from First Principles by Force Matching** — CHRISTOPHER JOHN<sup>1</sup>, THOMAS SPURA<sup>1</sup>, SCOTT HABERSHON<sup>2</sup>, ●DAVID E. MANOLOPOULOS<sup>2</sup>, and THOMAS D. KÜHNE<sup>3</sup> — <sup>1</sup>Institute of Physics, Johannes Gutenberg University Mainz, Staudinger Weg 9, D-55128 Mainz, Germany — <sup>2</sup>Physical and Theoretical Chemistry Laboratory, Oxford University, South Parks Road, Oxford OX1 3QZ, United Kingdom — <sup>3</sup>Institute of Physical Chemistry and Center for Computational Sciences, Johannes Gutenberg University Mainz, Staudinger Weg 9, D-55128 Mainz, Germany

We have applied the ring polymer molecular dynamics (RPMD) method [1,2] to investigate the effects of nuclear quantum effects of liquid water from first principles. Due to the fact that direct ab-initio RPMD simulations would be computational far too expensive, a flexible water potential is parameterized on forces from DFT-based Car-Parrinello-like MD simulations [3]. Initial results of RPMD simulations to determine static as well as dynamic properties of liquid water at ambient conditions using the so derived effective potential are presented and the importance of nuclear quantum effects are discussed.

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We have applied the ring polymer molecular dynamics (RPMD) method [1,2] to investigate the effects of nuclear quantum effects of liquid water from first principles. Due to the fact that direct ab-initio RPMD simulations would be computational far too expensive, a flexible water potential is parameterized on forces from DFT-based Car-Parrinello-like MD simulations [3]. Initial results of RPMD simulations to determine static as well as dynamic properties of liquid water at ambient conditions using the so derived effective potential are presented and the importance of nuclear quantum effects are discussed.

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