

## CPP 43: P8: Nanoparticles and Composite Materials

Time: Wednesday 10:00–13:00

Location: Poster A

CPP 43.1 Wed 10:00 Poster A

**The Effect of preparation method on the physical properties and the dynamic glass transition of the nanocomposites based on hyperbranched polymers** — ●SHEREEN OMARA<sup>1</sup>, MONA ABDEL REHIM<sup>2</sup>, AHMED GHONEIM<sup>3</sup>, SHERIF MADKOUR<sup>1</sup>, GAMAL TURKY<sup>3</sup>, and ANDREAS SCHÖNHALS<sup>1</sup> — <sup>1</sup>Federal Institute for Materials Research and Testing (BAM), Unter den Eichen 87, D-12200 Berlin, Germany — <sup>2</sup>Packing and Packaging Materials Department, National Research Center, Cairo, Egypt — <sup>3</sup>Microwave Physics and Dielectrics Department, National Research Center, Cairo, Egypt

Broadband dielectric spectroscopy, Specific heat spectroscopy, and Differential scanning calorimetry (DSC) are combined to study the glass transition and segmental motions in hyperbranched polyamine ester (HB PAE) and its nanocomposite with kaolinite (Ka). In situ polymerization and solution mixing (Ex situ) are applied to prepared HB-PAE/Ka nanocomposites with different concentrations of Ka. The dielectric spectra are dominated on the lower frequency (higher temperature) side by conductivity contribution. The molecular dynamic is found to be screened out by the conductivity contribution; otherwise Specific heat spectroscopy was used to determine the dynamic glass transition temperature of HBPs/Ka nanocomposite. The segmental motion related to the glass transition called alpha process found to play a role in the charge transport. The result indicated that the dc conductivity and the dynamic glass transition temperature depend not only on different concentrations of kaolinite but also on the method of the preparation of the nanocomposite.

CPP 43.2 Wed 10:00 Poster A

**Positioning of magnetic particles in polymer matrices for smart material engineering by magnetically patterned exchange bias templates** — ●IRIS KOCH<sup>1</sup>, MARKUS LANGNER<sup>2</sup>, ANDREAS GREINER<sup>2</sup>, and ARNO EHRESMANN<sup>1</sup> — <sup>1</sup>Department of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSA-T), University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel — <sup>2</sup>Department of Macromolecular Chemistry II, University of Bayreuth, Universitätsstr. 30, D-95440 Bayreuth

Magnetic micro-stripe patterned exchange bias systems with different stripe widths were used as a template for the precise positioning of either pure ferromagnetic nanoparticles or superparamagnetic core-shell microspheres in polymer thin film systems. The positioning was assisted by an out-of-plane magnetic field superimposing the magnetic field landscape of the exchange bias substrate. The particle/polymer composite was subsequently obtained via lift-off from the magnetically patterned template. An interaction with external magnetic fields was observed in air and in liquid environment down to a mass fraction of 3 % magnetic material in relation to the polymeric material.

CPP 43.3 Wed 10:00 Poster A

**Thermoelectric thin films based on a polymer/nanoparticle nanocomposite** — ●NITIN SAXENA<sup>1,2</sup>, ANTON GREPPMAIR<sup>3</sup>, MICHAEL CORIC<sup>4</sup>, JAN WERNECKE<sup>5</sup>, STEFANIE MARGGRAF<sup>5</sup>, EVA M. HERZIG<sup>4</sup>, MARTIN S. BRANDT<sup>3</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,2</sup> — <sup>1</sup>TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — <sup>2</sup>Center for NanoScience, LMU München, 80539 München, Germany — <sup>3</sup>TU München, Walter-Schottky-Institut and Physik-Department, 85748 Garching, Germany — <sup>4</sup>TU München, Munich School of Engineering, 85748 Garching, Germany — <sup>5</sup>Physikalisch-Technische Bundesanstalt, BESSY II Helmholtz-Zentrum Berlin, 12489 Berlin, Germany

Thermoelectric materials transform temperature gradients into voltages which can be used to generate electrical power. Highly efficient thermoelectrics comprise rare and/or toxic inorganic materials and require cost- and energy-intensive fabrication processes. This impedes their large-scale application for power generation.

In order to overcome these limitations, we pursue a hybrid approach combining the semiconducting polymer blend PEDOT:PSS for its high electrical conductivity and inorganic nanoparticles in order to reduce thermal conductivity within the thin film. We investigate the influence of the nanoparticles on the morphology of the blend by means of GISAXS and attempt to correlate this with changes in the thermoelectric behavior. Apart from that, we also investigate the thermal conductivity of both pristine PEDOT:PSS and of the hybrid film, in

order to ultimately calculate the figure-of-merit ZT.

CPP 43.4 Wed 10:00 Poster A

**Structural study of magnetic nanoparticle-block copolymer hybrid films prepared by printing techniques** — ●SENLIN XIA, YUAN YAO, EZZELDIN METWALLI, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Metal-polymer nano-composites are an important class of hybrid materials due to their interesting functional applications, e.g. sensors, and memory devices [1,2]. Hybrid films of magnetite nanoparticles and the diblock copolymer (DBC) poly(styrene-*b*-methyl methacrylate) are prepared using a printing method, with the potential of high mass production and energy saving. The relationship between viscosity of nanoparticle-polymer solution and the film formation was carefully explored in order to find the optimized processing conditions. The printed hybrid films are investigated using both real-space and reciprocal-space techniques. The nano- and microstructure of maghemite nanoparticles within DBC films as a function of the nanoparticle concentration is investigated using optical microscopy, atomic force microscopy, scanning electron microscopy and grazing incidence small-angle X-ray scattering. The magnetic property of the hybrid films is probed using a superconducting quantum interference device (SQUID) magnetometer. The observed structures are explained in the framework of microphase separation and confinements. A comparison of the nano-morphology between the spin-coated and printed hybrid films is discussed. [1] Y. Yao, et.al. ACS Appl. Mater. Interfaces 6, 5244, (2014); [2] Y. Yao et.al. ACS Appl. Mater. Interfaces 6, 18152, (2014).

CPP 43.5 Wed 10:00 Poster A

**Structure-Property relationships of Nanocomposites Based on Poly lactide and Layered Double Hydroxides** — ●JING LENG<sup>1</sup>, DE-YI WANG<sup>2</sup>, ANDREAS THÜNEMANN<sup>1</sup>, FRANZISKA EMMERLING<sup>1</sup>, ANDREAS WURM<sup>3</sup>, CHRISTOPH SCHICK<sup>3</sup>, and ANDREAS SCHÖNHALS<sup>1</sup> — <sup>1</sup>BAM Federal Institute for Material Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany — <sup>2</sup>IMDEA Materials Institute, C/Eric Kandel 2, 28906 Getafe, Madrid, Spain — <sup>3</sup>University of Rostock, Institute of Physics, Wismarsche Str. 43-45, 18051 Rostock, Germany

Two kinds of Polymer based nanocomposites prepared by melt blending of synthesized NiAl (NiAl-LDH) and MgAl (MgAl-LDH) layered double hydroxides with polylactide (PLA) were investigated by a combination of differential scanning calorimetry (DSC), small- and wide-angle X-ray scattering (SAXS and WAXS) and broadband dielectric spectroscopy (BDS). By detailed colorimetric investigations (stepscan DSC) the rigid amorphous phase due to the both the crystals and the nanoparticles was estimated unambiguously. A higher rigid amorphous fraction (RAF) due to the nanoparticles exists in the case of MgAl-LDH based nanocomposites compared to NiAl-LDH based nanocomposites. The dielectric spectra of the both nanocomposites showed several relaxation processes related to dynamic glass transition and localized fluctuations that were identified and analyzed in detail.

CPP 43.6 Wed 10:00 Poster A

**Structure-Property relationships of Nanocomposites Based on Epoxy and Layered Double Hydroxides** — ●JING LENG<sup>1</sup>, FRANZISKA EMMERLING<sup>1</sup>, DE-YI WANG<sup>2</sup>, and ANDREAS SCHÖNHALS<sup>1</sup> — <sup>1</sup>BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany — <sup>2</sup>IMDEA Materials Institute, C/Eric Kandel 2, 28906 Getafe, Madrid, Spain

Two kinds of organically modified MgAl Layered Double Hydroxides (MgAl-LDH) were synthesized and reaction blended with an epoxy system (EP) to obtain polymer based nanocomposites. The organic modification of the MgAl-LDHs were by sodium dodecylbenzene sulfonate (SDBS) modified and own synthesized nanofiller (SACC). The two kinds of nanocomposites were investigated by a combination of differential scanning calorimetry (DSC), small- and wide-angle X-ray scattering (SAXS and WAXS), and broadband dielectric spectroscopy (BDS) in dependence of the concentration of the nanofiller. The differences observed for the both kinds of nanoparticles are discussed in detail.

CPP 43.7 Wed 10:00 Poster A

**Morphology investigation of self-assembly of metal oxide-diblock copolymer nanocomposite films** — ●YUAN YAO<sup>1</sup>, EZZELDIN METWALLI<sup>1</sup>, JEAN-FRANCOIS MOULIN<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>HZ Geesthacht at FRM II, Lichtenbergstr.1, 85748 Garching, Germany — <sup>3</sup>Walther-Meissner-Institut, Walther-Meissner-Str. 8, 85748 Garching, Germany

The arrangement of maghemite nanoparticles (NPs) in diblock copolymer poly(styrene-*d*8-block-*n*-butyl methacrylate) P(S<sub>d</sub>-*b*-BMA) films via a self-assembly process is investigated. This study is motivated by great interests for many potential applications in functional nanodevices. The resulting hybrid thin films show a perforated lamella structure with an enrichment layer containing different NPs concentrations (from 0 up to 15 wt%) as investigated with X-ray reflectometry, scanning electron microscopy, atomic force microscopy, and grazing incidence small angle neutron scattering in time-of-flight mode (TOF-GISANS). The surface modified NPs are selectively positioned in one polymer domain at low NP concentrations and the microphase separation process is even enhanced in this case. However, a distortion of the lamella structure evolves with increasing NP concentrations.

CPP 43.8 Wed 10:00 Poster A

**Polymer metal oxide hybrid materials and films** — ●MICHAEL BAHR, EZZELDIN METWALLI, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching

Materials with novel electrical, optical and magnetic properties are possible thanks to the implementation of metal-polymer nanocomposite (MPN) structures. In future, thin films of MPN will be suitable for applications like sensors and memory devices. In such composites diblock copolymers are the matrix of choice for providing the desired arrangement of the metal, since they exhibit structure formation due to micro phase separation. Metal attaches preferentially to one of the two copolymer blocks, thereby forming a well-ordered structure inside the polymer matrix.

In this work we use an in-depth investigation of the system poly(styrene-*b*-methylmethacrylate) (PS-*b*-PMMA), which forms a lamellar structure, and a Cobalt salt based on a 2,2' bipyridine ring (C<sub>10</sub>H<sub>8</sub>Cl<sub>2</sub>CoN<sub>2</sub>). Bulk samples and thin films are prepared with different molar ratios of the salt and block copolymer by solution casting and by spin coating, where the cobalt content oxidizes. Bulk samples are characterized with in-situ thermal SAXS. Thin films are investigated with FTIR, AFM and SEM. We observe a well-ordered structure of the polymer matrix and a change of morphology with different molar ratios.

CPP 43.9 Wed 10:00 Poster A

**Gastransport Properties and Molecular Mobility of Matrimid/PhenethylPOSS Nanocomposites** — ●NORA KONNERTZ, MARTIN BOEHNING, and ANDREAS SCHOENHALS — BAM Federal Institute of Materials Research and Testing, Unter den Eichen 87, 12205 Berlin

Polymers are favored materials for gas separation membranes. The development of new material with higher permeabilities and selectivities is challenging because the structure and property optimization follows a trade-off: improvements of permeability is often connected to a reduction in selectivity and vice versa. A promising approach for improvements is the incorporation of nanoscaled fillers. In order to understand thus induced changes in the solution-diffusion mechanism (which describes the gas transport through polymer membranes) in more detail it is important to relate the molecular mobility of the polymer in the nanocomposites with the gas transport properties. Here this relation is studied using Matrimid5218 as polymer matrix and a polyhedral oligomeric silsesquioxane with phenethyl substituents (Phenethyl-POSS) as nanofiller. Films with filler contents up to 20 wt% were casted from dichloromethane solution (thicknesses around 100 μm). The molecular mobility is determined by broadband dielectric spectroscopy. Permeabilities were measured with the time-lag method (0 - 20 bar) and sorption by using a microbalance (0 - 45 bar) for different gases.

CPP 43.10 Wed 10:00 Poster A

**QCM System for the Characterization of Gas Sorption and Physical Aging on Membrane Polymers and Nanocomposites for Gas Separation Applications** — ●NORA KONNERTZ and MAR-

TIN BOEHNING — BAM Federal Institute of Materials Research and Testing, Unter den Eichen 87, 12205 Berlin

The Quartz Crystal Microbalance (QCM) is a very sensitive method to detect mass changes in a range of nanograms. Thus this method enables sorption experiments with thin films or layers attached to the QCM crystal (in a range up to 1 μm). Here we present the experimental set-up for using the QCM technique for characterizing the gas sorption behavior of thin polymer films in a temperature controlled pressurized environment (up to 50 bar). The piezoelectric quartz crystal is driven by a frequency controlled AC voltage. Mass changes of the oscillating system result in a frequency shift and changes of the conductance is monitored by a network analyzer and calibrated based on the Sauerbrey equation. The study aims for the characterization of long-term behavior and physical aging of high-performance polymers for gas separation membranes - such as polyimides and polymers of intrinsic microporosity (PIMs) and respective nanocomposites. Especially the differences of the behavior of thin films compared to films with thicknesses up to 100 μm as well as nanofiller induced-effects have to be investigated.

CPP 43.11 Wed 10:00 Poster A

**MUSIC mode AFM imaging of polystyrene-grafted functionalized graphene oxide** — ●MARTIN DEHNERT<sup>1</sup>, EIKE-CHRISTIAN SPITZNER<sup>1</sup>, FABIAN BECKERT<sup>2</sup>, CHRISTIAN FRIEDRICH<sup>2</sup>, and ROBERT MAGERLE<sup>1</sup> — <sup>1</sup>Chemische Physik, Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Germany — <sup>2</sup>Freiburger Material Forschungszentrum, Albert-Ludwigs-Universität, Freiburg, Germany

We investigate the surface morphology and the nanomechanical properties of organophilic stearylamine-modified graphene oxide (Stearyl-GO) sheets and a polystyrene-grafted functionalized graphene oxide (PS-*g*-FG) [1] using atomic force microscopy (AFM) operated in multi-set point intermittent contact (MUSIC) mode and force spectroscopy mode. This allows for depth-resolved mapping of the nanomechanical properties of the top surface layer of the functionalized graphene oxide (GO) sheets. On Stearyl-GO, we can distinguish areas of hydrophilic GO from hydrophobic stearylamine functionalized grafted areas. Exposure of PS-*g*-FG to chloroform vapor causes a selective-swelling and therefore a softening of the organic components stearyl and PS. This allows imaging the shape of the GO sheets embedded within the PS envelope. The GO sheets are folded and buckled in the PS envelope. The combination of swelling and MUSIC mode AFM imaging provides a detailed insight into the microstructure of functionalized GO sheets.

[1] Beckert F. et al.; *Macromolecules*, 2013, 46, 5488-5496

CPP 43.12 Wed 10:00 Poster A

**Drug Carriers based on HPMA Nanoparticles: Molar Mass and Buffer Type** — ●BART-JAN NIEBUUR<sup>1</sup>, NATALYA VISHNEVETSKAYA<sup>1</sup>, EKATERINA LOMKOVA<sup>2</sup>, PETR CHYTL<sup>2</sup>, SERGEY FILIPPOV<sup>2</sup>, and CHRISTINE M. PAPADAKIS<sup>1</sup> — <sup>1</sup>Fachgebiet Physik weicher Materie, Physik-Department TU München, Garching — <sup>2</sup>Institute of Macromolecular Chemistry, Prague, Czech Republic

A promising way to achieve site-specific delivery of anticancer agents is using the enhanced permeation and retention (EPR) effect of N-(2-hydroxypropyl) methacrylamide (HPMA) nanoparticles containing the drug doxorubicin (Dox) [1]. The present research in this field focuses on exploration of the particle structure and tuning of their properties. Recently, addition of different types of cholesterol and degradation of the linkage is used to tune the size and stability of these nanoparticles in dependence on pH [1].

The aim of the present study is to investigate the influence of molar mass of the HPMA backbone. Using fluorescence correlation spectroscopy (FCS), the size of the nanoparticles with and without Dox as well as the critical micelle concentration (CMC) are determined in a phosphate buffer. Investigation of the polymers containing Dox is challenging because of its broad own fluorescence emission. Moreover, more realistic environments are investigated. For instance, the conditions inside the bloodstream can be mimicked using serum.

[1] Filippov, K. et al., *Biomacromolecules* 14, 4061 (2013).

CPP 43.13 Wed 10:00 Poster A

**Metal Nanoparticle Growth on Model Homopolymer Thin Films** — ●VIVIAN WACLAWEK<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>2</sup>, GONZALO SANTORO<sup>2</sup>, JOHANNES F.H. RISCH<sup>2</sup>, SHUN YU<sup>3</sup>, TORSTEN BOESE<sup>2</sup>, PAUL STANIEC<sup>4</sup>, NICK J. TERRILL<sup>4</sup>, and STEPHAN V. ROTH<sup>1</sup> — <sup>1</sup>University of Hamburg, Luruper Chaussee 149, 22761 Hamburg — <sup>2</sup>DESY, Notkestr. 85, 22607 Hamburg — <sup>3</sup>KTH, Teknikringen 56-58, 10044 Stockholm — <sup>4</sup>DLS, Harwell Science and Innovation Campus,

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Nanostructured noble metal films on polymer layers are of fundamental importance in the field of organic electronics. Moreover, such material combinations have recently gained importance for stabilizing thin polymer films. We combine sputter deposition with grazing incidence X-ray scattering (GISAXS) to investigate in-situ [1-3] the growth kinetics of Au on polymethylmethacrylate. We analyze quantitatively the metal nanoparticle layer growth and compare our results with the metal layer structure on different model homopolymer films [4]. [1] Schwartzkopf et al., *Nanoscale* 5, 5053 (2013). [2] Yu et al., *J. Phys. Chem. Lett.* 4, 3170 (2013). [3] Santoro et al., *Appl. Phys. Lett.* 104, 243107 (2014). [4] Roth et al., *Appl. Phys. Lett.* 88, 021910 (2006).

CPP 43.14 Wed 10:00 Poster A

**Nanocomposites in High-Voltage Applications** — ●STEFAN O. HUBER<sup>1</sup>, ANNIKA REMPE<sup>2</sup>, BRUNO JAKOBI<sup>3</sup>, JURIY PACHIN<sup>2</sup>, MATTHIAS GRÜBEL<sup>3</sup>, JOHANNES SEILER<sup>2</sup>, JOSEF KINDERSBERGER<sup>2</sup>, BERNHARD RIEGER<sup>3</sup>, and GERALD J. SCHNEIDER<sup>1</sup> — <sup>1</sup>Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science & Institute of Complex Systems, 52425 Jülich, Germany — <sup>2</sup>Department of Electrical, Electronic and Computer Engineering, Institute for High Voltage Engineering and Switchgear Technology Arcisstr. 21, 80333 Munich, Germany — <sup>3</sup>WACKER-Chair of Macromolecular Chemistry, Lichtenbergstr. 4, 85748 Garching, Germany

Polymer based nanocomposites may exhibit enhanced electrical insulating properties. If we add silica nanoparticles to polydimethylsiloxane, we can see in the high voltage arc resistance test that the silica nanoparticles improve the material behavior.

Our poster aims to identify the origin of the increased arc resistance in silica nanocomposites and the dependence on different parameters such as the silica-volume-fraction, the molecular mass of the polymer and in changing the modification of the nanoparticles.

We produce silica nanocomposites and by different measurements, e.g. SAXS and SANS, we characterize the microscopic behavior. From these results we want to find a model to describe the macroscopic behavior, i.e. the resistance to high voltage arcing.

CPP 43.15 Wed 10:00 Poster A

**Morphology of nanocomposite copolymer electrolytes for Li+/polymer batteries** — ●KONSTANTINOS N. RAFTOPOULOS, MAJID RASOOL, EZZELDIN METWALLI, PETER MÜLLER-BUSCHBAUM, and CHRISTINE M. PAPADAKIS — TU München, Physik-Department, Fachgebiet Physik weicher Materie/LS Funktionelle Materialien, Garching

Long scale, effective transition to green energy and wide penetration of electric and hybrid cars, demand for batteries with high energy and power density, good mechanical stability, as well as impact and temperature resistance. Of crucial importance for the power density and the mechanical stability is the electrolyte component. Poly(ethylene oxide) (PEO) has proven itself as a reliable electrolyte, but it has two significant drawbacks: 1) Its crystallinity, while providing some stability, acts as a barrier to the mobility of the Li cations. 2) It lacks adequate dimensional stability, especially if mixed with Li+ salts. We use a block copolymer of PEO with polystyrene (PS) in order to provide dimensional stability, and we add SiO<sub>2</sub> nanoparticles to further enhance mechanical stability and suppress crystallinity. The morphology of the system is studied by X-ray scattering diffraction covering a large q-range, corresponding to multiple length scales, in order to study microphase separation and crystallinity.

CPP 43.16 Wed 10:00 Poster A

**Growth and disintegration of silver nanowires in tubular J-aggregates** — ●EGON STEEG, FRANK POLZER, HOLM KIRMSE, YAN QIAO, JÜRGEN P. RABE, and STEFAN KIRSTEIN — Institut für Physik, Humboldt-Universität zu Berlin

The reduction of AgNO<sub>3</sub> in the presence of tubular J-aggregates is used to prepare silver nanowires with 7 nm in diameter and lengths exceeding micrometers [1]. Here, we report on the influence of chloride ions on growth and dissolving of the wires. In presence of oxygen and a ligand the chloride ions are able to etch silver nanostructures by oxidizing neutral silver atoms back to ions [2]. This oxidative etching is more effective along defect zones than on defect free single crystals. Silver nanowires grown in the template structures are dissolved by addition of NaCl by this process and the silver is converted into AgCl while the tubular template is conserved. The dissolution of the Ag nanowires is explained by their structure which shows multiple twin

boundaries. The transport of the oxidized Ag atoms is explained by transport across the tubular wall.

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

[2] Y. Zheng et al., *Chem. Mater.* 2014, 26, 22-33

CPP 43.17 Wed 10:00 Poster A

**Adsorption of small polar and non-polar molecules on silica-nanoparticles** — ●CHRISTINA BALLNUS, SANDRA KATERNDAHL, JAN MEYER, and REINHARD HENTSCHKE — Bergische Universität, 42279 Wuppertal, Germany

A technically important application of nano particles is their use as filler materials in rubber compounds, e.g. in the tire industry. The latter employs both soot and silica, where silica is boosted by recent EU regulations for new tires aimed at improved wet grip, rolling resistance and noise reduction. The mechanical properties of filled rubber materials are very significantly affected by the interaction of the filler with the polymer matrix. Using computer simulations based on the Metropolis Monte Carlo technique in conjunction with the charge equilibration method, we have studied the adsorption of small molecules relevant to the above industry on silica nano particles at different temperatures. We obtain the site energy distribution depending on the nano particle's surface structure and size. This we compare to experimentally obtained adsorption energy distributions. We discuss how these results may be used in simulations aimed at the prediction of dynamic moduli of silica filled rubber.

CPP 43.18 Wed 10:00 Poster A

**SAXS and NEXAFS characterization of dispersions with magnetic nanoparticles (ferrofluids)** — ●CHRISTIAN GOLLWITZER<sup>1</sup>, RAUL GARCIA DIEZ<sup>1</sup>, MICHAEL KRUMREY<sup>1</sup>, and NORBERT BUSKE<sup>2</sup> — <sup>1</sup>Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, 10587 Berlin, Germany — <sup>2</sup>MagneticFluids, Berlin, Köpenicker Landstrasse 203, 12437 Berlin, Germany

Ferrofluids contain magnetic nanoparticles (like magnetite or maghemite) with superparamagnetic properties [1]. Aqueous ferrofluids with different crystal sizes between 5 nm and 10 nm (TEM) and hydrodynamic diameters between 20 nm and 200 nm (DLS) were prepared. On the one hand, the particles were electrostatically stabilized towards aggregation showing a high positive zeta potential. On the other hand, the particles were covered with fruit acids (i.e. citrate) indicating a negative zeta potential at a neutral pH value.

SAXS and NEXAFS measurements were carried out at the four-crystal monochromator (FCM) beamline of PTB at the synchrotron radiation facility BESSY II in Berlin to determine the mean size and size distribution of the primary particles, the size and fractal dimension of the agglomerates and the oxidation state of the nanoparticles. It was found, that the used ferrofluids are stable for at least several months from preparation.

[1] ROSENSWEIG, R. 1987 Magnetic fluids. *Ann. Rev. Fluid Mech.* 19, 437-463

CPP 43.19 Wed 10:00 Poster A

**Modeling of the phase separation behavior of nanocomposites from blockcopolymers and nanoparticles in thin films - Comparing theoretical and experimental results** — ●PETER FRIEDEL, DORIS POSPIECH, DIETER JEHNICHEN, ASTRID DRECHSLER, PETRA UHLMANN, and ANDRIY HORECHYY — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden

Thin films from nanocomposites containing polymer blends or block-copolymers and nanoparticles allow manifold applications in the generation of specific surface structures with tailor-made properties. Theoretically considered, these are three component systems with specific periodic boundary conditions. The resulting three component spinodal hypersurfaces calculated by meanfield calculations makes one able to guess the symmetry of the microphase separated structures and the distribution of the nanoparticles within the thin films. The theoretical results of two different specific copolymer systems should be compared with experimental findings. Firstly, a system containing a fixed bottom PNiPAAM layer including an dense layer of hydrophized Fe<sub>3</sub>O<sub>4</sub> nanoparticles and an additional top layer with different polymers (containing either PMMA, P2VP or PS) was investigated as a example for polymer blend/nanoparticle composite. Secondly, a system with a PMMA-PPMA diblock copolymer including Au nanoparticles or Fe<sub>3</sub>O<sub>4</sub> nanoparticles was investigated as an example for diblock copolymer/nanoparticle composite.

CPP 43.20 Wed 10:00 Poster A

**Periodic plasmonic nanoparticle arrays with controllable interparticle distances and plasmon resonance coupling** — ●KIRSTEN VOLK and MATTHIAS KARG — Physical Chemistry I, University of Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany

Surface plasmons (SPs) are light induced collective oscillations of the electron liquid in respect to the crystal lattice at a metamaterial-dielectric interface with permittivities of different signs. When employing nanoparticles with a size smaller than the skin depth, optical fields can penetrate its entire volume and drive localized surface plasmon oscillations. The plasmon resonance wavelength of metallic nanoparticles is highly dependent on the size, shape and the material of the nanoparticle. Additionally the localized surface plasmon resonance (LSPR) is sensitive to the dielectric environment and the interparticle distance in nanoparticle arrays. Varying these two parameters significant changes of the optical properties of the system due to coupling can be achieved.

In this contribution we show how to make use of the dielectric environment and interparticle distance dependence of LSPRs to create functional materials with tailored optical properties. As particular building blocks we employed silver nanoparticles, which are coated by a polymer shell. The particles are then self-assembled into highly ordered hexagonally packed monolayers by a floatation approach. The interparticle distances can be exactly tuned by the dwell-time of the particles at the liquid-air interface. By placing the monolayers on substrates with high refractive indices the optical properties of the system can be further enhanced.

CPP 43.21 Wed 10:00 Poster A

**Charge Storage in  $\beta$ -FeSi<sub>2</sub> Nanoparticles** — JENS THEIS<sup>1</sup>, ●SEBASTIAN KÜPPER<sup>1</sup>, ROBERT BYWALEZ<sup>2</sup>, HARTMUT WIGGERS<sup>2</sup>, and AXEL LORKE<sup>1</sup> — <sup>1</sup>Fakultät für Physik and CENIDE, Universität Duisburg-Essen — <sup>2</sup>Institut für Verbrennung und Gasdynamik and CENIDE, Universität Duisburg-Essen

The increasing use of mobile electronics creates a steady demand for new energy storages with very high capacitance. Here we report on the observation of a surprisingly high specific capacitance of  $\beta$ -FeSi<sub>2</sub> nanoparticle layers. The devices work without the need of a fluid phase, the charge storing material is abundant and cost effective, and the sample design is easy to fabricate. Lateral, interdigitated capacitor structures were fabricated on thermally grown silicon dioxide and covered by FeSi<sub>2</sub> particles by drop or spin casting. The FeSi<sub>2</sub>-nanoparticles, with sizes in the range of 10-30 nm, were fabricated by gas phase synthesis in a hot wall reactor. Compared to the bare electrodes, the nanoparticle-coated samples exhibit a 3-4 orders of magnitude increased capacitance. Time-resolved current voltage measurements show that for short times (seconds to minutes), the material is capable of storing up to 1 As/g at voltages around 1 V. The devices are robust and exhibit long term stability under ambient conditions. The specific capacitance is strongly dependent on the air humidity. It is highest for a relative humidity of 95%, while for a relative humidity below 40% the capacitance is almost indistinguishable from a nanoparticle-free reference sample. An isotope effect can be observed by using heavy water vapour.

CPP 43.22 Wed 10:00 Poster A

**Influence of additives on the structure of CTAB and its role in gold nanoparticle formation** — ●TILO SCHMUTZLER, TORBEN SCHINDLER, MARTIN SCHMIELE, and TOBIAS UNRUH — Friedrich-Alexander-University Erlangen-Nuernberg, Chair for Crystallography and Structural Physics, Staudtstrasse 3, 91058 Erlangen, Germany.

Au nanoparticles (NPs) have been the subject of widespread research in the last two decades. Therefore, numerous studies dealing with the synthesis leading to exact shape and size control were made. Applications are expected in biological imaging, drug delivery and phototherapeutics.[1]

The common wet chemical synthesis of anisotropic Au NPs is the seed-mediated growth synthesis route.[1] Therefore small seed particles are used to grow nanorods in a solution of CTAB (Cetyltrimethylammonium bromide) as structure directing agent.

The behaviour of CTAB in solution and so the influence on the final Au NP formation can be influenced by additives like alcohols or inorganic salts. Increasing concentrations of KBr for example lead to a higher repulsion of the micelles which was investigated by small angle X-ray and neutron scattering (SAXS, SANS) whereas UV-Vis spectroscopy revealed a slower formation kinetic of the Au NPs in KBr containing CTAB solutions. The characterization of the final Au NPs

via SAXS and transmission electron microscopy (TEM) show systematic variations of the particle dimensions.

[1] C.J. Murphy et al., J. Phys. Chem B. 2005, 109, 13857-13870.

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**Effective Interaction between globular, multivalent target-inhibitor-systems** — ●SUSANNE LIESE<sup>1</sup>, JONATHAN VONNEMANN<sup>2</sup>, DANIEL LAUSTER<sup>3</sup>, SUMATI BATHIA<sup>2</sup>, ANDREAS HERRMANN<sup>3</sup>, ROLAND R. NETZ<sup>2</sup>, and RAINER HAAG<sup>1</sup> — <sup>1</sup>Freie Universität Berlin, Institut für theoretische Physik — <sup>2</sup>Freie Universität Berlin, Institut für Chemie und Biochemie — <sup>3</sup>Humboldt Universität zu Berlin, Institut für Biologie

Multivalency is an important design principle in nature. It is based on the simultaneous binding of several relatively weak binding partners, in order to strengthen the over-all interaction[1]. In our project we focus in on the interaction of globular, multivalent target-inhibitor-systems, as they are found in virus-inhibition-assays[2]. In these systems the target/inhibitor is evenly covered with receptor-/ligand-binding sites. The resulting interaction is influenced by the collective binding of multiple receptor-ligand-pairs as well as by geometric shielding due to the extended size of target and inhibitor. We use a combination of coarse grained simulations and analytical methods to study the influence of the particle size, receptor/ligand-density and geometric shielding on the effective binding constant. [1] M. Mammen, S. Choi, G. M. Whitesides, *Angew. Chem. Int. Ed.* 1998, 37, 2754-2794 [2] I. Papp, C. Sieben, A.L. Sisson, J. Kostka, C. Böttcher, K. Ludwig, A. Herrmann, R. Haag, *ChemBioChem* 2011, 12, 887-895

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**SPONTANE TRANSFORMATION VON POLYELEKTROLYTSTABILISIERTEN SILBERNANOPRISMEN DURCH INTERAKTION MIT KSCN** — ●ANDREA KNAUER und J. MICHAEL KÖHLER — Technische Universität Ilmenau, Fak. Mat. Nat., Inst. f. Chemie und Biotechnologie, Gustav-Kirchhoffstr. 1, 98693 Ilmenau

Die Reaktion von kolloidalen Silbernanoprismen mit Rhodanidionen resultiert in einer spontanen Transformation der flachen, lateral ausgedehnten Nanoprismen in kompakte, sphärische Nanopartikel. Diese Reaktion kann nicht durch ein einfaches Ätzen der Dreiecksspitzen erklärt werden, wie es vielfach in der Literatur in Bezug auf die Reaktion mit bspw. Halogenidionen beschrieben wird. Unter beschriebenen Reaktionsbedingungen werden bei der spektralphotometrischen in-situ Überwachung isobestische Punkte beobachtet, die darauf hinweisen, dass die Formumwandlung von einer Spezies in die andere auf direktem Weg, ohne Ausbildung von Intermediaten, geschieht. Die beobachteten Reaktionskinetiken des Umwandlungsprozesses können mithilfe eines Ansatzes der molekularen Konversion besser beschrieben werden als durch einen Prozess mit stufenweisem Transport von Material. Die Interpretation der Befunde hat hohe Signifikanz bezüglich des allgemeinen Verständnisses von formanisotropen Edelmetallnanopartikeln: Die Silber-Nanodreiecksprismen werden durch ihre spezifischen elektronischen Eigenschaften und der Interaktion mit einem oder wenigen Polyelektrolytmolekülen stabilisiert und erscheinen eher als molekular-analoges System statt als kleine Festkörper.

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**Specific detection of molecules with NanoSPR** — ●SIRIN CELIKSOY<sup>1</sup>, RUBÉN AHIJADO-GUZMÁN<sup>1</sup>, ANDREAS HENKEL<sup>1</sup>, JANAK PRASAD<sup>1,2</sup>, CHRISTINA ROSMAN<sup>1</sup>, GERMÁN RIVAS<sup>3</sup>, and CARSTEN SÖNNICHSEN<sup>1</sup> — <sup>1</sup>Institute of Physikal Chemistry, University of Mainz, Germany — <sup>2</sup>Graduate School Materials Science in Mainz, University of Mainz, Germany — <sup>3</sup>Centro de Investigaciones Biológicas, Madrid, Spain

Nanoparticles hold potential to be used in multiplexed, inexpensive, fast medical diagnostic assays, e.g. for the identification of novel influenza strains. Common approaches for parallel analyte detection in small liquid samples link specific receptor molecules to spectrally encoded markers, thus limiting the number of targets in a parallel assay to a few dozen. Micro-spot arrays where targets bind in pre-defined positions could overcome these limitations. However, current multiplexed detection schemes are too complex, slow and/or expensive for routine use in the point-of-care environment. We show a new approach to detect multiple analytes simultaneously in a microfluidic flow cell using randomly deposited gold nanorods. Each nanorod responds with a spectral shift of its plasmon resonance specifically to one target, acting effectively as a NanoSPR device. Here, we demonstrate the feasibility of the concept, its sensitivity in the nanomolar range, sensor reusability

over consecutive cycles, and the potential for up-scaling the concept. Our technique has the potential to simplify multiplexed detection and substantially reduce the costs of production, especially if combined with advanced nanofabrication methods.

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**Energy transfer characteristics of Mn doped CdS/ZnS quantum dots** — UWE KAISER<sup>1</sup>, MIKKO WILHELM<sup>1</sup>, JOHANNES RÖDER<sup>1</sup>, NADEEM SABIR<sup>1</sup>, LORENZ MAXIMILIAN SCHNEIDER<sup>1</sup>, PABLO DEL PINO<sup>2</sup>, CAROLINA CARRILLO-CARRION<sup>1</sup>, WOLFGANG PARAK<sup>1</sup>, and WOLFRAM HEIMBRODT<sup>1</sup> — <sup>1</sup>Department of Physics, Philipps University Marburg, Germany — <sup>2</sup>CIC Biomagune, San Sebastian, Spain

Core shell CdS/ZnS quantum dots (QDs) doped with manganese in the ZnS shell are investigated. Photoluminescence spectra show the successful doping of the ZnS shell by the identification of the typical

Mn luminescence band around 580nm. Time resolved measurements confirm this additionally by determination of the long lifetime (2ms) for this spin forbidden transition. By doping the CdS/ZnS QDs we obtain a system with two very distinct luminescence bands around 450nm from the CdS core and around 580nm from the manganese ions. The energy transfer between these two luminescence centers is not only determined by the spectral position of both bands but additionally by the interface between CdS and ZnS within the QD. The results lead furthermore to the conclusion that the low energetic Mn state cannot only act as acceptor for the high energetic CdS transition, but vice versa also as donor. This leads to an enhanced CdS lifetime from hundreds of ns without Mn to several ms in the case of Mn doping. Measurements of Mn doped QDs and QDs additionally functionalized by dye molecules also show a lifetime of the dye in the ms range, due to energy transfer from the excited Mn.