

and precise location, including also that of the counter charge.

### 15 min. break

CPP 41.7 Thu 15:45 H48

**Synthesis of stable bimetallic AuAg and CoPd colloids via diblock copolymer micelle nanoreactors** — ●WILLIAM G. MENEZES<sup>1</sup>, VOLKMAR ZIELASEK<sup>1</sup>, CHRISTIAN KÜBEL<sup>2</sup>, KARSTEN THIEL<sup>3</sup>, and MARCUS BÄUMER<sup>1</sup> — <sup>1</sup>Universität Bremen, Institut für Angewandte und Physikalische Chemie — <sup>2</sup>Forschungszentrum Karlsruhe / KIT — <sup>3</sup>Fraunhofer IFAM, Bremen

The preparation of metal nanoparticles (NPs) by using block copolymers (BCP) as encapsulating agent yields NPs with narrow size distributions and outstanding control over the inter-particle distance. Various metal salts, also in combination, can be easily loaded as precursor for NPs into the micelle cores.[1] We will demonstrate the synthesis of AuAg and CoPd bimetallic NPs by using PS-*b*-P4VP as stabilizing agent and N<sub>2</sub>H<sub>4</sub>·H<sub>2</sub>O as reducing agent. TEM images show spherical crystalline NPs with diameters varying between 3 and 6 nm, for both, AuAg and CoPd. In UV-vis only one plasmon band at 460 nm was observed for Au-Ag NPs, indicating the formation of truly bimetallic NPs. STEM and EDX confirm that single NPs contain both metals, in the case of AuAg with atomic ratios of Au:Ag as 1:1, in agreement with the metal salt concentrations used. In catalysis, bimetallic systems can demonstrate unique properties distinct not only from the bulk metals but also from the corresponding monometallic NPs. The results of first catalytic tests for CO oxidation at titania loaded with AuAg and CoPd NPs prepared via the BCP route will be presented. Despite the organic matrix, the NPs are active for CO oxidation under certain conditions.

[1] S. Förster, M. Antonietti, Adv. Mater. 10 (1998) 195.

CPP 41.8 Thu 16:00 H48

**Hybrid raspberry particles for superhydrophobic surfaces** — ●DORIS VOLLMER, MARIA D'ACUNZI, LENA MAMMEN, and HANS-JÜRGEN BUTT — Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz (Germany)

On superhydrophobic surfaces, water droplets roll off even at inclinations of just a few degrees, taking up any contaminants encountered on their way. In nature, the lotus leaf is one of the most efficient examples of a superhydrophobic surface. Its superhydrophobicity is conferred by surface roughness on the nano- and micrometer scale.

Here we report a novel method to prepare superhydrophobic films from raspberry particles. The term \*raspberry particle\* refers to the topography of their surfaces with nano-sized secondary spheres attached to a considerably larger primary particle. Our particles consist of a polystyrene core and a rough silica shell. The hybrid nature of our particles offers the possibility to design a completely new approach to prepare superhydrophobic surfaces.

Multilayers of particles are formed by evaporation of the aqueous dispersant. By exposure of the hybrid particles to tetrahydrofuran vapour, polystyrene leaks out of the core and forms bridges between the particles, thereby providing mechanical stability. The films are hydrophobized by silanization with a semifluorinated silane. Films show static contact angle for water of about 160° and roll-off angle of 1°.

CPP 41.9 Thu 16:15 H48

**Electron beam-induced nanoparticle formation in Au and Pt salt-loaded polystyrene-block-poly(4-vinylpyridine) micelles** — ●VOLKMAR ZIELASEK<sup>1</sup>, CHRISTIAN KÜBEL<sup>2</sup>, WILLIAM G. MENEZES<sup>1</sup>, KARSTEN THIEL<sup>3</sup>, and MARCUS BÄUMER<sup>1</sup> — <sup>1</sup>Universität Bremen, Institut für Angewandte und Physikalische Chemie — <sup>2</sup>Forschungszentrum Karlsruhe/KIT — <sup>3</sup>Fraunhofer IFAM, Bremen

Using diblock copolymer micelles as nanoreactors for the generation of metal colloids has proven to be a universal route to regular arrays of uniformly sized nanoparticles (NPs) for a variety of metals [1]. When PS-*b*-P4VP micelles in toluene are loaded with metal salts, the formation of a single NP in each P4VP core can be achieved in a subsequent reduction step induced either chemically, by plasma or by UV or electron irradiation. We will present a detailed TEM study of metal colloid formation during this reduction step in Au and Pt salt-loaded PS-*b*-P4VP micelles at variable temperature in the range 95 - 300 K. Electron irradiation-induced coagulation of metal and initial formation of particulates with subnanometer diameters within the P4VP cores is observed in the entire temperature range for Au as well as for Pt. Particle coarsening and ripening, however, strongly depend on the

metal, the electron dose and, in particular, on temperature. Counter-intuitively, the dynamics of metal aggregation into a single NP within each micelle core is faster at low temperature whereas at 300 K even high densities of subnanometer particulates remain stable. Stability of the P4VP is probably essential for metal mobility within the core.

[1] S. Förster, M. Antonietti, Adv. Mater. 10 (1998) 195.

CPP 41.10 Thu 16:30 H48

**Ground state structures in ferrofluid monolayers: influence of an external magnetic field** — ●TAISIA PROKOPIEVA<sup>1</sup>, VICTOR DANILOV<sup>1</sup>, SOFIA KANTOROVICH<sup>1,2</sup>, and CHRISTIAN HOLM<sup>2</sup> — <sup>1</sup>Ural State University, Ekaterinburg, Russia — <sup>2</sup>ICP, University of Stuttgart, Stuttgart, Germany

More and more attention is given to ferrofluid monolayers recently because they find different applications in various disciplines. Based on our previous results [Prokopyeva et al. Phys. Rev. E (2009), V.80, P. 031404], we investigate the microstructure of ferrofluid thin films at low temperatures under applied external magnetic field. Using a combination of analytical methods and Monte Carlo simulations we have studied the ground state structures in two cases: the field aligned perpendicular and parallel to the layer. The crucial influence of the external field is demonstrated. We find different configurations for different magnetic fields. The critical parameters of structural transitions for different fields are proved to depend on the number of particles in the system.

The results of the ground state structures in the presence of the external field will be used to understand the microstructure of ferrofluid monolayers at room temperatures.

CPP 41.11 Thu 16:45 H48

**Ferrofluids With Shifted Dipoles** — ●RUDOLF WEEBER, SOFIA KANTOROVICH, JOAN J. CERDÀ, and CHRISTIAN HOLM — Institute for Computational Physics, Pfaffenwaldring 27, 70569 Stuttgart, www.icp.uni-stuttgart.de

In the last decades, ferrofluids and magnetic colloids have become relevant in many applications ranging from engineering to medicine, and therefore have attracted the interest of scientists from many fields. We present simulations and analytical calculations for a model system for magnetic nanoparticles that have a dipole moment shifted out of the center of mass, towards the surface. I.e., the spherical symmetry of the particle is broken. This model is inspired by experiments on colloidal particles with magnetic caps by Erbe et al. While it does not attempt to reproduce the experiments exactly, similar structures can be observed already for intermediate shifts of the dipole. In our contribution, we discuss ground state properties for small clusters, which help us to understand the building blocks of larger systems. For moderate shifts of the dipole moment, the ground state structure changes from chains and rings with parallel alignment of moments, usually observed in dipolar particles, to pairs and triangles with close to anti-parallel orientation of moments. We also present magnetization properties of larger systems at finite temperature and observe the influence of the shift in particular on the initial slope of the magnetization curve, namely, the initial susceptibility.

CPP 41.12 Thu 17:00 H48

**Molecular Dynamics Simulations of Thermal Decomposition of Methane using a Reactive Force Field** — ●NORBERT LÜMMEN — University of Bergen, Department of Physics and Technology, Allégaten 55, 5007 Bergen, Norway

Incomplete combustion of carbon based materials produces fine carbon rich particles. Controlled manufacturing of very pure carbon nanoparticles (Carbon Black) can be achieved by, for example, thermal decomposition of gaseous precursors like acetylene or methane.

Molecular dynamics simulations of hydrocarbon growth after non-catalyzed thermal decomposition of methane were carried out in order to understand the impact of the thermal decomposition reaction of methane on the formation of large hydrocarbon molecules and their role in formation of carbon nanoparticles [1]. A reactive force field (ReaxFF [2]) was employed to model the interactions of the involved hydrocarbons.

After thermal decomposition of methane the formation of molecular hydrogen, a broad range of hydrocarbons and carbon dimers was observed. The basic reactions are in agreement with existing models of thermal decomposition of methane. An increasing variety of hydrocarbons is observed with increasing temperature. The largest molecules formed within 1 ns of simulation time contain enough carbon atoms to be able to form 5- or 6-membered carbon ring structures.