# CPP 13: Poster: Nanoparticles, Nanocrystals and Composites

Time: Monday 18:15–21:00 Location: Poster B2

CPP 13.1 Mon 18:15 Poster B2

**Study of silica nanoparticles/polymer hydrogel nanocomposite** — •Elsa Perrin[1,2], Martin Schoen[1,3], and Anne Boutin[2] — [1]Stranski-Laboratorium für Physikalische und Theoretische Chemie, Fakultät für Mathematik und Naturwissenschaften, Technische Universität Berlin, Berlin, Germany — [2]Ecole Normale Supérieure, PSL Research University, UMR PASTEUR, Paris, France — [3]Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, North Carolina, USA.

The design of nanocomposite materials is a fast-growing field with many novel and exciting materials such as nanocomposite polymer hydrogels. In particular, the coupling between the chemistry of adsorption and the resulting mechanical properties has been poorly explored. Recently a way has been found to glue together two polymer gels using nanocomposite materials made by polymers and silica nanoparticles (NPs). It is proposed for the first time that spreading a droplet of a silica NP solution on the surface of one gel and then bringing a second gel into contact with it leads to strong adhesion between the two gels.

However, the interaction between the polymer network and the NPs is still not well understood. Modeling the interactions between polymers and silica particles at the quantum level, using density functional theory, will allow us to get insight into the adsorption energy of the polymers on the NPs surface. Moreover, studying this system with coarse-grained molecular dynamics simulations will give us information about the organization of the polymer chains around the silica NPs.

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**Porous titania-based hybrid films as electrodes for lithium-ion batteries** — •Thomas Kaps, Ezzeldin Metwalli, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Porous titania films are promising candidates as electrodes for lithium-ion batteries. Large surface area of nanoporous titania films enables both, high current density and improved cycling behavior. Sol-gel templating is nowadays a widely used technique to create nanoscale porous structures. PS-b-PEO diblock copolymer is used as a structure directing agent to create foam-like mesoporous titania/silicon composite films via sol-gel method. The morphology of the porous hybrid films was probed with SEM, X-ray diffraction and GISAXS. The crystallinity of the titania films was systematically measured as a function of the silicon nanoparticle content following the calcination step at different temperatures. The titania/silicon hybrid films are tested as electrodes for lithium-ion batteries showing a unique combination of both, the high capacity and the resistance to the lithium dendrites formation.

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**Printed nanostructured block-copolymer/metal-oxide hybrid films** — •Senlin Xia, Ezzeldin Metwalli, Yuan Yao, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Metal-polymer nanocomposites are important hybrid materials due to their interesting applications, e.g. catalysts, sensors, and memory devices. Owing to the potential of high mass production and energy saving, printing techniques were utilized to prepare hybrid films composed of magnetite nanoparticles (NPs) and PS-b-PMMA diblock copolymer (DBC). Different external magnetic fields were applied during the printing process to guide the NPs within the polymer matrix. The mesoscopic structure of PS-coated maghemite NPs within the DBC films was investigated as a function of the NP concentration using optical microscopy, AFM, SEM and GISAXS. The PS-coated NPs were selectively dispersed in the PS domains of the parallel lamella NP-DBC hybrid films. At high NP concentrations, the coalescence of NPs into large micro-sized metal-oxide wires was observed. The superparamagnetic behavior of the hybrid film was proved using a superconducting quantum interference device magnetometer.

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**Magnetic properties and structure of block copolymer-cobalt oxide nanocomposite thin films** — •Hong Xu, Ezzeldin Metwalli, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Nanostructured polymer-metal oxide composites are a current research area of great importance due to its highlight applications in sensors, optics and catalysts. In the present investigation, the structure and properties of hybrid films composed of a PS-b-PMMA diblock copolymer (DBC) and cobalt metal salt were investigated. Cobalt metal salt oxidation in the polymer matrix was probed with UV/Vis and FTIR spectroscopies during the thermal treatment step. The interdomain lamella spacing D was evaluated using GISAXS as a function of cobalt salt concentration. The D values increased with an increasing of Co/PMMA molar ratios. Both, paramagnetic and superparamagnetic behavior of the heat-treated hybrid films were proved at different cobalt salt contents using superconducting quantum interference device magnetometer.

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**Numerical studies of acoustic metamaterial multilayers** — •Takamichi Terao — Gifu university, Gifu, JAPAN

The vibrational properties of acoustic metamaterial multilayers, which are made of a periodic arrangement of clusters of mass and mass-in-mass microstructure, were numerically studied. The dispersion relations of one-dimensional multilayers and two-dimensional periodic structures with square lattices were clarified. It was confirmed that flat modes appear in a sonic band gap, and that the number of such in-gap modes can be controlled by changing the structure of a multilayer. The physical origin of the flat modes is also discussed.

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**Strong correlated electronic system in Mn3+ oxide revealed by RIXS** — •Daniela Schön, Ronny Golnak, Marc F. Tesch, Jie Xiao, and Emad F. Aziz — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Deutschland

MnOx has been demonstrated as effective water oxidation catalysts, among which Mn3+ species has been proven as the most efficient ingredient when compared to other Mn oxidation states. The information on electronic structure of MnOx is certainly critical to understand the catalytic mechanism and to further improve the catalytic activity. While most of the electronic structure investigations are conducted on solid samples, few are performed in liquid environment to mimic realistic conditions. We selected solvated Mn3+acac3 in dichloromethane as a prototypical system to carry out in-situ RIXS measurements, an ideal model system probed by a proper technique. Mn3+ ion is coordinated by six O atoms in liquid phase, which perfectly simulates the situation of Mn3+ species during water catalysis. RIXS is able to detect element-specific valence excitations in bulk, an ideal tool to probe local (catalytic site) electronic structure of Mn in liquid. Moreover, the intensity ratio of RIXS loss features to normal emission features can be utilized to determine the extent of the electronic correlation in the target system. Intense RIXS loss features of Mn3+ are observed, implying a highly localized and strong correlated electronic system in Mn3+ d4 configuration.

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**Molecular Dynamics Simulations of a Peptide Modified Silica Nanopore** — •Kai Stroh, Julian Geske, and Michael Vogel — Institut für Festkörperphysik, TU Darmstadt

The combination of biological and synthetic nanopores is of great biotechnological interest. While being highly selective and sensitive, biological nanopores lack the robustness for technological applications. In contrast silica pores are well-proven in industrial and clinical environments, but possess inferior capabilities, e.g. no selectivity. A hybrid system would combine the favourable properties of both fields.

To investigate the interactions between biological chain molecules attached to mesoporous materials and various liquids, we employ molecular dynamics simulations. For our peptide modified silica system we chose a slit pore geometry. Elastin-mimetic peptides $(\mathrm{VPGVG})_\mathrm{n}$ are grafted onto the two surfaces of a silica slab via suitable linker molecules. The intergallery space is filled with aqueous mixtures. We study how the configuration of the peptide changes in the vicinity of a silica surface and how the behavior of the water mixtures is affected by the confinement. Moreover, we investigate the dynamical couplings of peptide and solvent molecules.

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**Mechanical properties of molecularly covered silver nanowires investigated by SFM** — •Katherine A. Herman[1], Egon Steeg[1], Jürgen P. Rabe[1,2], and Stefan Kirstein[1] — [1]Department of Physics, Humboldt Universität zu Berlin — [2]IRIS Adlershof, Humboldt Universität zu Berlin

Silver nanowires with uniform diameters of 6.5 nm were deposited onto solid substrates and investigated using scanning force microscopy (SFM). The wires were synthesized using an established protocol[1] with a soft tubular molecular aggregate template in aqueous solution. Filled and unfilled tubule segments could best be discriminated by the phase contrast of the intermittent contact SFM imaging mode. Contact mode SFM was used to move, bend and break deposited tubules with and without silver wires. Analysis of the broken and dragged segment lengths suggests that the wires break preferentially at certain grain boundaries, as expected for a polycrystalline material. Analysis of the wire conformations indicates that the wires were plastically deformed during deposition.

[1] D. M. Eisele, H. v. Berlepsch, C. Böttcher, K. J. Stevenson, D. A. Vanden Bout, S. Kirstein, J. P. Rabe. *J. Am. Chem. Soc.*, 2010, 132**(7)**, pp 2104-2105.

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**Novel Growth Mechanism of ZnO Hexagonal Microtube Optical Resonators** — •Jinxin Zhan[1], Hongxing Dong[1], Shulin Sun[2], Xiaodong Ren[3], Jianjun Liu[3], Zhanghai Chen[2], Chritoph Lienau[4], and Long Zhang[1] — [1]Shanghai Institute of Optics and Fine Mechanics, 201800 Shanghai, China — [2]Fudan University, 200433 Shanghai, China — [3]Shanghai Institute of Ceramics, 200050 Shanghai, China — [4]Carl von Ossietzky Universität, 26111 Oldenburg, Germany

Tubular micro/nanostructures have gained considerable interest for both fundamental scientific studies and practical applications due to their unique and delicate constructions [1-2]. However, for quite a long time, it was quite difficult to synthesize tubular structures for non-layered materials such as oxides, metals and nitrides because of the difficulties of controlling their dimensions.

Here we observed a novel growth mechanism of tubular ZnO microstructures. As demonstrated by a detailed growth study of ZnO crystals and by first-principles calculations, the formation of $H_2/H_2O$ vapour changes the ZnO crystal surface energy and controls the geometry of ZnO micro/nanotubes.Furthermore, we demonstrated that the fabricated microtubes could be employed as tunable optical resonators. The effect of the unique tubular structure on the intensity modulations is discussed theoretically based on a plane wave model and finite-element-method (FEM) simulations, which agrees well with the experimental results.

[1] J. Xu et al., Adv. Mater. 26, 5337 (2014); [2] H. X. Dong et al., J. Mater. Chem. 20, 5510 (2010)

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**Studying visible-light photodegradation of Benzidine azo dye on Titanium dioxide nanotubes using Surface Enhanced Resonance Raman Spectroscopy** — •Christine Joy Querebillo[1,2], Hoang Khoa Ly[1], Ibrahim-Halil Öner[1], Ulrich Gernert[3], Peter Hildebrandt[1], and Inez Marita Weidinger[1] — [1]Institut für Chemie, PC 14, Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany — [2]School of Analytical Sciences Adlershof, Humboldt-Universität zu Berlin, IRIS Building, Unter den Linden 6, 10099, Berlin, Germany — [3]Zentraleinrichtung Elektronenmikroskopie (ZELMI), Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany

Surface Enhanced Resonance Raman Spectroscopy (SERRS) is used to study the photodegradation of an azo dye pollutant, Benzidine-p-aminothiophenolate (BD-PATP), on Titanium dioxide (TiO2) nanotubes. Unlike many degradation studies on TiO2 which use UV light, here, we use visible light to photodegrade BD-PATP on TiO2 of different surface enhancements achieved with different post-anodization heat treatment temperatures (300-500°C). Heating the TiO2 nanotubes at these temperatures improves the crystallinity, as seen in Raman, and affects the morphology of the nanotubes, as seen using scanning electron microscopy.

SERRS was used to confirm the synthesis of BD-PATP on TiO2 from PATP on TiO2 and to monitor the photodegradation of BD-PATP on TiO2. For the latter, we infer on the effect of the surface enhancement of the nanotubes on the photodegradation kinetics.

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**Highly efficient energy transfer from quantum dot to allophycocyanin in hybrid structures** — •Anastasia Karpulevich[1,3], Evgeny Maksimov[1], Nikolay Sluchanko[2], Alexandr Vasiliev[1], and Vladimir Paschenko[1] — [1]Lomonosov Moscow State University, 119991, Moscow, Russia — [2]A.N.Bach Institute of Biochemistry, 119071, Moscow, Russia — [3]Institute of Physical Chemistry, Hamburg University, 20146, Hamburg, Germany

Development of light-energy converters based on photosynthetic mechanisms is one of the promising directions in modern biophysics. Quantum dots can be used as a substitution to the native light-harvesting antennae, increasing absorbtion cross-section of purified photosystem as a result of non-radiative energy transfer [1]. We investigated model system consisting of CdSe/ZnS core-shell quantum dot (QD) and protein allophycocyanin (APC). Using spectroscopic methods we shown that QD-APC hybrid systems are able to self-assemble in solution. We found that steric accessibility plays a key role for the energy transfer: the energy migration efficiency in hybrid structures reaches 90 % for APC monomers and only 30 % for trimers. Additionally, we obtained stable covalently bound QD-APC hybrids. We observed considerable amplification of APC fluorescence in the optical range of excitation between 400 and 500 nm, where QD absorption prevails. The results might be used for the creation of bright and stable fluorescent dyes based on allophycocyanin.

[1] E.G. Maksimov et al., Biochem., vol. **77**, no. 6, pp. 624*630 (2012).

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**Scanning aperture trapping of nanoparticles for plasmonic enhancement of fluorescence** — •Yazgan Tuna, Ji Tae Kim, and Vahid Sandoghdar — Max-Planck-Institute for the Science of Light, 91058 Erlangen

Trapping and manipulation of small objects have been of interest for a range of applications. Here we report on an electrostatic trap that is created in an aqueous medium between the aperture of a nanopipette and a glass substrate without the need for external potentials. Furthermore, we demonstrate scanning aperture trapping and manipulation of nanoparticles and study the plasmonic enhancement of fluorescence of a single fluorophore.

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**Preparation and physical characterization of magnetite nanoparticles (MNP) with Aminosilane shell** — •Maryam Youhannayee[1], Stanislav Emelianov[1], Robert Rabenalt[2], and Mathias Getzlaff[1] — [1]Institute für angewandte physik, Heinrich-Heine-universität Düsseldorf — [2]Klinik für Urologie, Universitätsklinikum Düsseldorf

Magnetite Nanoparticles are widely studied because of their fascinating application and also biocompatibility and low toxicity in different fields of biology and medicine. These nanoparticles covered with Aminosilane are perfect candidates for hyperthermia therapy due to a nearly perfect prevention of wash-out. In this contribution, the synthesis of magnetite nanoparticles by chemical coprecipitation is presented. In a first step, magnetite nanoparticles were prepared by coprecipitation of ****2+ and ****3+ with ammonium. Subsequently, magnetite nanoparticles were coated with a ligand shell consisting of Aminosilane. Different techniques were used for morphology and structure characterization. Dynamic light scattering technique was carried out to investigate the size distribution of nanoparticles in wet environment. TEM images also prove the formation of spherical MNP. For characterizing the crystal structure, X-ray diffraction was used. These measurements show that different parameters such as preparation speed have a significant influence on the size of nanoparticles.

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**Hot Brownian Motion** — •Alexander Fischer — Molecular Nanophotonics, Institut für Experimentalphysik I, Fakultät für Physik und Geowissenschaften, Universität Leipzig

Hot Brownian motion describes the motion of a heated microsphere in a liquid. A temperature field is created around the heated particle decaying with 1/r. The heat transferred from the particle to the surrounding fluid spreads around three orders of magnitude faster than the particle moves. Therefore a stationary temperature field is moving with the particle through the liquid. The non-equilibrium dynamics of the particle now differs from the unheated particles and an effective temperature and diffusion constant is introduced to describe the system. With the development of fast detection systems in the recent years and the possibility to restrict the motion of a microscopic object using an optical tweezer, an investigation of hot Brownian motion on short time scales has become possible. Due to the increasing impact of the particle's inertia and the surrounding fluid on short time scales, the motion of the particle is not completely random anymore. The aim of this research is to understand the fundamentals of an effective temperature definition for fluctuation dissipation relations under non-equilibrium conditions.