

## CPP 14: POSTERS Nanoparticles

Time: Tuesday 14:00–16:30

Location: P3

CPP 14.1 Tue 14:00 P3

**Energy Transfer on Molecular Aggregates** — ●JAN RODEN<sup>1</sup>, ALEXANDER EISEL<sup>1</sup>, and WALTER STRUNZ<sup>2</sup> — <sup>1</sup>MPI-PKS Dresden, Finite Systems — <sup>2</sup>TU Dresden, Theoretische Quantenoptik

Since the discovery in the 1930's, molecular aggregates have attracted experimental and theoretical research, due to their unique linear and non-linear optical properties [1]. Furthermore they are possible candidates for artificial light harvesting units.

The properties of such molecular aggregates are strongly affected not only by static disorder, but also by internal vibrations of the constituting monomers, which couple strongly to electronic excitation [2]. To understand the optical properties and the energy transfer dynamics of molecular aggregates a theory has to properly take into account these effects.

Using a new approach based on a non Markovian Schrödinger equation [3] allows the non-perturbative treatment of internal vibrational modes of the monomers which are coupled to the surrounding. The comparison with results obtained by direct diagonalization of a model Hamiltonian containing one vibrational mode per monomer shows good agreement. The influence of vibrations to the energy transfer is discussed.

[1] T. Kobayashi, (ed.) J-Aggregates, World Scientific, 1996

[2] A. Eisfeld, J. S. Briggs, Chem. Phys. 324, (2006) 376

[3] T. Yu, L. Diosi, N. Gisin, W. Strunz, Phys. Rev. A. 60, (1999) 91

CPP 14.2 Tue 14:00 P3

**About the active role of aluminum oxide nanoparticles on network formation in epoxy nanocomposite system: Influence of mixing sequence.** — ●BARTOSZ ZIELINSKI, MARTINE PHILIPP, ULRICH MÜLLER, PIERRE-COLIN GERVAIS, ROLAND SANCTUARY, JÖRG BALLER, and JAN KRISTIAN KRÜGER — LPM, University of Luxembourg, Luxembourg

Many properties of polymer nanocomposites can be significantly improved by adding appropriate fillers like nanoparticles. The desired features of the polymer nanocomposites can be achieved by the properties of the nanoparticles themselves and/or by interactions between the polymer matrix and the particles. Due to chemical and/or physical interactions between the nanoparticles and the polymer matrix the properties of the composite are often more affected than predicted, as such interactions lead to the creation of an additional morphology called interphase. The formation of interphases is often in concurrence with the bulk polymerization process. In consequence the mixing sequence of the nanoparticles and the other constituents of the nanocomposite can already have a strong impact on the final properties.

It will be shown that by optical investigations already in the primary suspensions (resin/nanoparticles and hardener/nanoparticles) significantly different properties and therefore different interactions are present. As a matter of fact the different optical properties do not vanish but even increase in the course of polymerization. Accordingly the network formation has to be influenced by the interactions, too.

Refractometry was chosen as experimental technique.

CPP 14.3 Tue 14:00 P3

**Photophysical studies of zinc porphyrin oligomers** — ●JĘDRZEJ SZMYTKOWSKI<sup>1,2</sup>, JONAS CONRADT<sup>1</sup>, WOLFGANG LÖFFLER<sup>1</sup>, TEODOR SILVIU BALABAN<sup>2,3</sup>, MATTHIEU KOEPPF<sup>4</sup>, JENNIFER WYTKO<sup>4</sup>, JEAN WEISS<sup>4</sup>, and HEINZ KALT<sup>1,2</sup> — <sup>1</sup>Karlsruhe Institute of Technology (KIT), Universität Karlsruhe (TH), Institute of Applied Physics, Karlsruhe, Germany — <sup>2</sup>Center for Functional Nanostructures (CFN), Karlsruhe, Germany — <sup>3</sup>Karlsruhe Institute of Technology (KIT), Forschungszentrum Karlsruhe, Institute for Nanotechnology, Karlsruhe, Germany — <sup>4</sup>Institut de Chimie, UMR 7177, Université Louis Pasteur, Strasbourg, France

The fabrication of novel multiporphyrinic arrays is important for the progress of molecular electronics and to mimic self-assembling chromophores in artificial light harvesting devices. We report on the time resolved photoluminescence studies of two novel phenanthroline strapped Zn-porphyrins having an imidazole pendant arm and C<sub>12</sub> or C<sub>18</sub> alkyl chains. The luminescence dynamics have been analyzed using decay associated spectra (DAS). The obtained results show the formation of well-ordered J-aggregates. Such self-assembled species have been recently directly observed for these porphyrins deposited on

the mica surface by various nanoscopic techniques. No evidence of energy transfer from the phenanthroline strap to the zinc porphyrin has been found, a fact which can be explained by unfavourable Förster- and Dexter-type energy transfer processes.

CPP 14.4 Tue 14:00 P3

**Time resolved luminescence spectroscopy of self-assembling magnesium porphyrins** — ●JĘDRZEJ SZMYTKOWSKI<sup>1,2</sup>, JONAS CONRADT<sup>1</sup>, CHILLA MALLA REDDY<sup>3</sup>, TEODOR SILVIU BALABAN<sup>2,3</sup>, and HEINZ KALT<sup>1,2</sup> — <sup>1</sup>Karlsruhe Institute of Technology (KIT), Universität Karlsruhe (TH), Institute of Applied Physics, Karlsruhe, Germany — <sup>2</sup>Center for Functional Nanostructures (CFN), Karlsruhe, Germany — <sup>3</sup>Karlsruhe Institute of Technology (KIT), Forschungszentrum Karlsruhe, Institute for Nanotechnology, Karlsruhe, Germany

Self-assembled porphyrins are promising materials to mimic natural bacteriochlorophylls (BChl) *c*, *d* or *e* encountered in the chlorosomes of photosynthetic bacteria. Such large assemblies of porphyrin metal complexes can be also used in hybrid solar cells as light harvesting antennas. In order to address their suitability we have studied the time resolved luminescence of novel magnesium diacetyl porphyrins. The decays of luminescence have been analyzed by a fitting procedure, which produces decay associated spectra (DAS). The analysis shows a short-lived component associated with the supramolecular architecture. This has implications for optimizing device geometries where the exciton diffusion lengths are not surpassed.

CPP 14.5 Tue 14:00 P3

**Magnetische Eigenschaften Mn-dotierter CdSe/CdS-Halbleiternanopartikel bei thermischer Behandlung** — ●ANDREAS HOFMANN<sup>1</sup>, SHIH-HAO KUNG<sup>1</sup>, CHRISTINA GRAF<sup>1</sup>, KRISCHAN JELTSCH<sup>1</sup>, CHRISTINE BOEGLIN<sup>2</sup> und ECKART RÜHL<sup>1</sup> — <sup>1</sup>Inst. f. Chemie u. Biochemie, Freie Universität Berlin, 14195 Berlin — <sup>2</sup>Inst. de Physique et Chimie d. Matériaux de Strasbourg, 67034 Strasbourg

Mn-dotierte CdSe/CdS-Nanomischkristalle mit variabler Mn-Konzentration und einem Durchmesser von 2.9-3.8 nm wurden mit chemischen Hochtemperaturverfahren synthetisiert. Im Anschluss daran wurden die Partikel bei 210 °C für 48-72 h in Hexadecylamin getempert. Um die elektronische Struktur und die magnetischen Eigenschaften der Mn-Atome während dieser Erhitzungsphase näher zu untersuchen, wurden an den Partikeln magnetische Röntgenzirkulardichroismus-Messungen durchgeführt.[1] Dabei wurde untersucht, inwieweit hierbei eine Änderung des paramagnetischen Verhaltens erfolgt und ob eine lokale Mn-Se-Mn-Clusterbildung auftritt.[2] Die durchgeführten Messungen zeigen eine Änderung des Spinmoments nach dem Tempern infolge der veränderten lokalen Umgebung des Mn. Dabei konnte gezeigt werden, dass der Syntheseprozess den Temper-Effekt deutlich beeinflusst. Ein in Ref. [2] diskutierter Übergang des Mn vom paramagnetischen hin zum superparamagnetischen Verhalten konnte jedoch für diese Systeme ausgeschlossen werden, da keine oder nur eine unvollständige Clusterbildung stattgefunden. [1] A. Hofmann et al. Chem. Phys. Chem. 8, 2008 (2007). [2] D. Magana et al. J. Am. Chem. Soc. 128, 293 (2006).

CPP 14.6 Tue 14:00 P3

**Spectroscopic fingerprints of photodegrading CdSe/ZnS quantum dots** — ●DANNY KOWERKO, JÖRG SCHUSTER, and CHRISTIAN VON BORCZYKOWSKI — Center of nanostructured materials and analytics, TU-Chemnitz, 09107 Chemnitz

Colloidal semiconductor nanocrystals have been under investigation for more than a decade with a growing field of applications in science and industry. However, photophysics and chemistry are still not fully understood, since crystal structure of core and shell as well as ligands may vary slightly between different charges, thus yielding individual optical properties even of single quantum dots from the same stock. We will discuss the role of surface (states) and its defined modification (e.g. by functionalized dye molecules) with special regard to nanocrystal degradation processes which are obviously accompanied by distinct spectral shifts and lifetime alterations. Besides time resolved ensemble studies in solution, we have chosen a multiparameter single particle approach, giving insight to spectral and luminescence lifetime fluctuations of individual quantum dots. Comparison of individual - on SiO<sub>2</sub> immobilized - untreated and modified species will provide a deeper

insight towards the underlying mechanisms of surface manipulation induced photodegradation and thus allow for a correlation with the ensemble results.

CPP 14.7 Tue 14:00 P3

**Sidewall functionalization of carbon nanotubes for preparation of nanocomposites** — ●ANASTASIA GOLOSOVA<sup>1,2</sup>, GERHARD RICHTER<sup>2</sup>, ANDREAS TIMMANN<sup>3</sup>, RAINER JORDAN<sup>2</sup>, and CHRISTINE PAPADAKIS<sup>1</sup> — <sup>1</sup>TU München, Physikdepartment, Garching — <sup>2</sup>TU München, Department Chemie, Garching — <sup>3</sup>HASYLAB at DESY, Hamburg

In polymer nanocomposites, the nanometer size active fillers can change the material properties of polymer matrices within a wide range. Among others, carbon nanotubes (CNTs) are some of the most intriguing additives due to their unique mechanical, thermal, and electrical properties. However, until now the challenge of efficient incorporation and compatibilization of the CNTs with the surrounding matrix, which is crucial for the anticipated improved properties of the composite, is still unsolved.

To tune the surface properties of CNTs we extended a recently developed modification to form well-defined self-assembled monolayers from (bi)phenyl diazonium salt derivatives on carbon-based substrates to the sidewall modification of CNTs. Successful covalent functionalization of the nanotubes was confirmed by Raman spectroscopy and thermo-gravimetric analysis.

In order to investigate the dispersion ability of modified samples, we performed SAXS experiments (HASYLAB at DESY). Intensive scattering from big agglomerates of raw carbon nanotubes in deionized water was observed, while the dispersions of modified CNTs were homogeneous, which confirms better solubility of functionalized samples.

CPP 14.8 Tue 14:00 P3

**Characterization of optical active nanostructures on silicon** — ●THOMAS BAUMGÄRTEL, HARALD GRAAF, and CHRISTIAN VON BORCZYSKOWSKI — Center of Nanostructured Materials and Analytics, TU Chemnitz, 09107 Chemnitz, Germany

Anchoring optically active molecules on nanostructured surfaces is a promising step towards building complex structures with variable properties and functions. Recently we could demonstrate that nanostructures on silicon surfaces can be functionalized in a neat way through selective binding of dye molecules and nanoparticles [1]. Here we report on the characterization of nanostructures on silicon that have been optically functionalized by binding of cationic dye molecules. The nanostructures were created by AFM-induced local anodic oxidation of dodecyl-terminated silicon. The two cationic dyes rhodamine 6G and cresyl violet have been selectively attached to nanostructures via electrostatic interactions and were studied using wide-field and confocal microscopy. The spectrum of the bound dyes indicates the existence of two different species of molecules: some of the molecules show the same spectral emission compared to dye molecules in solution, for other molecules there is a clear blue-shift of the emission wavelength. The bleaching behaviour of the dyes on to the structure follows a biexponential decrease pointing also towards two different species of bound dyes.

[1] H. Graaf, M. Vieluf, and C. von Borczyskowski, *Nanotechnology* 18, 265306 (2007)

CPP 14.9 Tue 14:00 P3

**Mechanical properties of self-assembled mesoscale fibers investigated by AFM bending experiments** — ●DANIEL KLUGE<sup>1</sup>, FRANK ABRAHAM<sup>2</sup>, STEPHAN SCHMIDT<sup>1</sup>, HANS-WERNER SCHMIDT<sup>2</sup>, and ANDREAS FERY<sup>1</sup> — <sup>1</sup>Department of Physical Chemistry II, University of Bayreuth, Universitätsstraße 30, 95440 Bayreuth, Germany — <sup>2</sup>Department of Macromolecular Chemistry I, University of Bayreuth, Universitätsstraße 30, 95440 Bayreuth, Germany

Fibers with diameters in the range of nm to  $\mu\text{m}$  have a large field of applications, mainly for tissue engineering and in composite materials. However, little is known about the mechanical properties of individual fibers on the mesoscale. We used AFM (atomic force microscopy) for force measurements in analogy to a macroscopic 3 point bending test to investigate self-assembled fiber-like structures of aromatic benzene trisamides. These had the ability to form remarkable hexagonal hollow cylinder morphologies. Our results suggest that their elastic modulus is comparable to semi-crystalline polymers. One special feature of our measurements was the usage of the force mapping mode of the AFM. This was a facile way to enhance the reliability of the measurements and collect significant amounts of data at the same time. The extensive

data collection of our method marks a good starting point for future modeling and a thorough understanding of single-fiber deformation on the mesoscale.

CPP 14.10 Tue 14:00 P3

**Molecular dynamics simulations of nucleation and growth of mixed  $\text{FeCl}_2/\text{NaCl}$  nanoparticles from supercritical water** — ●NORBERT LÜMMEN and BJØRN KVAMME — University in Bergen, Department of Physics and Technology, Allégaten 55, 5007 Bergen, Norway

Nanoparticle formation from single  $\text{Fe}^{2+}/\text{Na}^+/\text{Cl}^-$  ions in water at supercritical conditions was investigated by molecular dynamics (MD) simulations [1]. Systems with 2048  $\text{H}_2\text{O}$  rigid SPC/E water molecules and 120  $\text{Fe}^{2+}$  ions, 240  $\text{Cl}^-$  ions and additional either 24 or 72  $\text{Na}^+/\text{Cl}^-$  ion pairs were simulated at various state points. The water-ion and ion-ion interaction was treated by a combination of Coulomb and Lennard-Jones potentials. The temperature was controlled by a heat bath thermostat using the Nosé-Hoover mechanism on the water molecules.

The method of Yasuoka and Matsumoto [2] and the Mean First Passage Time method [3] were compared for obtaining nucleation rates and critical cluster sizes from the simulation data. We found good agreement between these methods. The nucleation rates increased with increasing NaCl amount while the critical cluster sizes decreased. We also investigated properties of the growing clusters like size, composition, structure and shape and their dependence on the state conditions.

[1] Lümmen, Kvamme, *Phys. Chem. Chem. Phys.* 10, 6405 (2008)

[2] Yasuoka, Matsumoto, *J. Chem. Phys.* 109, 8451 (1998)

[3] Wedekind et al., *J. Chem. Phys.* 126, 134103 (2007)

CPP 14.11 Tue 14:00 P3

**Optically Detected Cyclic Voltammetry on Single Semiconductor Quantum Dots** — ●ANGEL TOPALOV, NICOLE AMECKE, and FRANK CICHOS — Molecular Nanophotonics Group, Institute of Experimental Physics I, University Leipzig, Linnéstraße 5, 04103 Leipzig

An interesting and promising class of materials studied over the last years are semiconductor nanocrystals. Many applications seek to make use of their favorable fluorescence characteristics, like tunable emission wavelength, high quantum yield and photon statistics (antibunching). Additionally they show certain peculiarities like power-law blinking, lifetime-fluctuations and spectral diffusion which can be explained by charges close to or in the dot center leading to Auger processes (non-radiative energy transfer to those charges) and the quantum confined stark effect. Those charges can arise from ejection of electron or hole via tunneling leaving behind the counterpart and additionally changing the matrix charge constellation. One of the main ideas is, thus, the development of an experimental method and setup for controlling those charges on the single particle level, starting with a determination of the specific ionization energy and electron affinity of different sizes of quantum dots. We then use confocal microscopy and cyclic voltammetry (CV) together, which gives us remarkable opportunities for experimental observations on the influences of charges on single crystal fluorescence.

CPP 14.12 Tue 14:00 P3

**Absorption and energy transfer of quantum aggregates** — ●JAN RODEN<sup>1</sup>, WALTER STRUNZ<sup>2</sup>, JOHN BRIGGS<sup>3</sup>, and ALEXANDER EISFELD<sup>1</sup> — <sup>1</sup>MPIPKS Dresden — <sup>2</sup>TU Dresden, Theoretische Quantenoptik — <sup>3</sup>Uni Freiburg, Theoretische Quantendynamik

The coupling of electronic excitation to vibrational degrees of freedom strongly influences characteristic properties of quantum aggregates (e.g. optical properties and energy transfer dynamics). We treat this exciton-phonon coupling using a non-Markovian stochastic Schrödinger equation [1]. Solving a Holstein-type model, we determine optical and transfer properties for exciton dynamics coupled to a realistic, complex phonon bath such that energy dissipation to the phonons is fully included. Our approach captures uniformly the transition from fully coherent to incoherent excitation transfer. As a specific example demonstrating the capability of this approach, we investigate J-band and H-band spectra and energy transfer dynamics of mesoscopic molecular aggregates. The results are compared with that of the well established CES approximation (Coherent Exciton Scattering [2]) and the exact solution for the extreme case when the complex spectral density is replaced by that of a single harmonic oscillator.

[1] T. Yu, L. Diosi, N. Gisin, W. Strunz, *Phys. Rev. A* 60, (1999) 91

[2] J.S. Briggs, A. Herzenberg *J. Phys. B* 3, 1663 (1970)

CPP 14.13 Tue 14:00 P3

**Raman Spectroscopic Study of Plasma Functionalized Carbon Nanotubes (CNTs)** — ●VERENA KATZENMAIER<sup>1,2</sup>, JAKOB P. BARZ<sup>1</sup>, NICOLAS P. ZSCHOERPER<sup>1,2</sup>, MICHAEL HAUPT<sup>1</sup>, UWE VOHRER<sup>1</sup>, CHRISTIAN OEHR<sup>1</sup>, and THOMAS HIRTH<sup>1,2</sup> — <sup>1</sup>Fraunhoferinstitut Grenzflächen- und Bioverfahrenstechnik, 70569 Stuttgart — <sup>2</sup>Institut Grenzflächenverfahrenstechnik, Universität Stuttgart

Raman spectroscopy is well known as a powerful tool for the characterization of carbon structures. In the case of CNTs, Raman spectroscopy provides a deep insight into their physical properties as well as the material quality. In resonance conditions, the Raman scattering process is strongly influenced by the electronic states of the system: in the case of single walled nanotubes, this is seen by e.g. the van Hove singularities.

In order to get a fundamental insight in structural properties and effects of chemical functionalization via low pressure plasma treatment, measurement conditions were varied in different ways: bulk material in the form of bucky papers was probed by a confocal system with three different excitation energies (e.g. 488 nm, 632.8 nm, 785 nm). In addition, the CNTs were measured with a tunable laser system in order to probe resonant scattering processes.

We focused on the low-frequency radial breathing mode for studying the nanotube diameter distribution of our samples as well as the conducting properties of the tubes.

CPP 14.14 Tue 14:00 P3

**A universal relationship concerning the mechanical properties of amorphous materials: the generalized Cauchy relation** — ●MARTINE PHILIPP<sup>1</sup>, ULRICH MÜLLER<sup>1</sup>, ROLAND SANCTUARY<sup>1</sup>, PATRICK ALNOT<sup>2</sup>, and JAN KRÜGER<sup>1</sup> — <sup>1</sup>LPM, University of Luxembourg, Luxembourg, Luxembourg — <sup>2</sup>LPMIA, University of Nancy, Nancy, France

Classical Cauchy relations (CR) are known for crystals from solid state physics. They reduce the number of independent elastic moduli compared to that given by point symmetry. From the theoretical viewpoint such CR are not expected for amorphous materials. However, a linear relationship between the longitudinal and shear elastic moduli  $c_{11}(x)$  and  $c_{44}(x)$ , called generalized CR (gCR)  $c_{11}(x) = 3c_{44}(x) + A$  ( $x$ : driving parameter), was observed for many amorphous materials at high probe frequencies. The Cauchy parameter  $A$  is a constant for a given material. Recently it has been shown that the gCR with the same parameter  $A$  holds even true when varying consecutively different parameters  $x$  (like temperature, chemical conversion). This implies that the independency of the elastic moduli is strongly reduced for a given material.

In this presentation the combination of the two parameters chemical conversion and different amount of nanoparticles will be discussed for a reactive epoxy/silica nanocomposite. A new interpretation of the gCR and its parameter  $A$  will be given in terms of the local morphology of the considered material. All investigations were performed by Brillouin spectroscopy.