## MM 49: Nanomaterials II: Synthesis

Time: Thursday 10:15-11:30

Location: H39

MM 49.1 Thu 10:15 H39 SOLIDIFICATION BEHAVIOUR OF INDIUM DROPLETS EMBEDDED IN AN ALUMINIUM MATRIX - • MOSTAFA Mohaned, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, Münster, Germany

A hypomonotectic alloy of Al- 0.5-4 at% In has been manufactured by the melt-spinning technique. The microstructures of the embedded nanoparticles were investigated by transmission electron microscopy (TEM). As-melt spun alloy of Al-In consists of a homogeneous distribution of faceted particles formed during the monotecitc solidification reaction.

The In nano-particles show a cube-cube orientation relationship with the surrounding Al-matrix. The kinetics of In particles solidification have been examined by heating and cooling experiments in a differential scanning calorimetry (DSC) over a range of heating and cooling rates. Analyses of the nucleation kinetics of In particles solidification have been performed in the frame of the classical spherical cap model of heterogeneous nucleation.

MM 49.2 Thu 10:30 H39

Optical Nanoparticle Sorting Elucidates Synthesis of Plas**monic Nanotriangles** — •Christoph Maier<sup>1</sup>, Maria A. Huergo<sup>2</sup>, Marcos F. Castez<sup>2</sup>, Carolina Vericat<sup>2</sup>, Roberto C. SALVAREZZA<sup>2</sup>, ALEXANDER S. URBAN<sup>1</sup>, and JOCHEN FELDMANN<sup>1</sup> <sup>1</sup>Chair for Photonics and Optoelectronics, Department of Physics, Ludwig-Maximilians-Universität, Amalienstaße 54, 80799 Munich, Germany — <sup>2</sup>Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas, Universidad Nacional de La Plata, Sucursal 4 Casilla de Correo 16, 1900 La Plata, Argentina

The synthesis of plasmonic nanoparticles by reducing gold salt by sodium sulfide leads to the formation of a strong near infrared (NIR) extinction peak [1], signifying strong potential for hyperthermic cancer treatment. However, the nature of the underlying nanoparticles has been a matter of debate. Hybrid core-shell and gold nanoparticles with different shapes have been discussed. [2] We introduce wavelength selective optical printing in order to sort the synthesized nanoparticles according to their plasmon resonances. By arresting the synthesis at different times, we find that thin gold nanotriangles are responsible for the observed NIR resonance. We also discuss and explain the observed spectral shifts of the plasmon resonances as observed during synthesis. This novel method is applicable to other plasmonic nanoparticle syntheses. In the future, complex nanostructures can be built up on substrates by selectively printing nanoparticles of varying plasmonic resonances. [1] Zhou, H.S., et al., PRB 1994, 50, (16), 12052-12056 [2] Diao, J. J., et al., J. Chem. Phys 2006, 124, (11), 116103

MM 49.3 Thu 10:45 H39

Carbon Dots: A Unique Fluorescent Cocktail of Polycyclic Aromatic Hydrocarbons — •FLORIAN EHRAT<sup>1</sup>, MING FU<sup>1</sup>, SAN-TANU BHATTACHARYYA<sup>1</sup>, YU WANG<sup>2</sup>, JACEK STOLARCZYK<sup>1</sup>, Andrey Rogach<sup>2</sup>, Alexander Urban<sup>1</sup>, and Jochen Feldmann<sup>1</sup> <sup>1</sup>Photonics and Optoelectronics Group, Department of Physics, Ludwig-Maximilians-Universität (LMU), Munich, Germany <sup>2</sup>Department of Physics and Materials Science, City University of Hong Kong, Hong Kong SAR

Carbon dots (CDs) have attracted rapidly growing interest due to their exceptional advantages such as high fluorescence quantum yield, chemical stability and biocompatibility. Recently the fluorescent CDs have been used for bioimaging, photocatalysis, photovoltaics, as lightemitting diodes, and for lasing. However, the intrinsic mechanism and origin of the fluorescence in CDs have not yet been completely understood.

We have recently developed a model system of polycyclic aromatic

hydrocarbon (PAH) molecules embedded in a polymer matrix to reproduce the optical properties of CDs.[1] In particular, a large Stokes shift of more than 100 nm as well as excitation wavelength dependent emission properties could be achieved by fine-tuning of the concentration of only three different molecules. Therefore we conclude that these can be seen as the main emissive species within a CD. These results will help to enable specifically tailoring the optical characteristics of CDs.

[1] M. Fu, F. Ehrat, et al., Nano Lett. 2015, 15 (9), 6030-6035.

MM 49.4 Thu 11:00 H39 Anodic aluminum oxide: regularity evolution with time, temperature and underlying aluminum structure — •Stefan Os-TENDORP, MARTIN PETERLECHNER, and GERHARD WILDE - Institute of Materials Physics, WWU Münster, 48149 Münster, Germany

Anodic aluminum oxide (AAO) has proven itself as a versatile tool for nano-structuring purposes. Its ability to form a regularly arranged hexagonal pore array renders its utilization as a template or mask for the fabrication of zero- and one-dimensional nanostructures possible. Ever since pre-structuring and multistep anodizations have been introduced to yield regular through-hole structures, AAO has been used for the synthesis of different functional surface nano-structures. However, AAO growth and especially the regularity evolution under certain anodization conditions remained impossible to explain in a comprehensive way. Thus we focus in this work on quantitative investigations of AAO's regularity evolution with anodization time, temperature and with respect to the structure of the aluminum, the AAOs have been anodized from, to derive conditions for regular pore formation. Based on advanced anodization control as well as a graphical regularity analysis, AAOs fabricated under mild and hard anodization conditions have been studied and compared. It has been found, that the aluminum grain size and orientation has only a minor effect on the AAO's regularity. Moreover, there is actually no temperature dependence of the obtained regularity at all. Finally the regularity evolution with time revealed an electrolyte degeneration being responsible for sudden regularity loss, which might have been misinterpreted in previous works.

## MM 49.5 Thu 11:15 H39

Computational study of fluorinated metal-organic frameworks applied to oil-water separation — •JAMES MORAES DE Almeida<sup>1</sup>, Caetano Rodrigues Miranda<sup>2</sup>, and Nicola Marzari<sup>1</sup> <sup>1</sup>THEOS and NCCR MARVEL, EPFL, Lausanne, Switzerland —  $^2 \mathrm{Nanopetro,}$ Instituto de Física, USP, São Paulo, Brazil

Metal-organic frameworks (MOFs) have high surface areas and no lost space due to non-accessible volumes. Selective adsorption of fluids in MOFs is highly dependent on their surface properties, leading to a variety of applications. One example is oil-water separation, where MOFs can selectively adsorb oil molecules but not water - which is important to clean oil spills. MOFs with this property have been synthesized, typically with fluorinated surfaces (FMOFs - fluorinated MOFs). In this work, we perform first-principle simulations to study the interactions of FMOFs with several adsorbates: anthracene, naphthalene, phenol, heptane, benzene, benzoic-acid, toluene, methane and water. The calculated binding energies show that, with an exception of the methane, all hydrocarbons have stronger binding to the FMOFs. In addition, we analyzed the location of the HOMO and LUMO orbitals. While the LUMO is never found on the adsorbate, the HOMO (or at least the HOMO-1) can sit on the molecules for several cases - anthracene, benzene, naphthalene, benzoic-acid and toluene - making these all available for chemical reactions. Last, while hydrocarbons interact strongly with FMOFs, water still has a favorable adsorption energy, but will be displaced by all the hydrocarbons considered, but methane.