

HL 71: New concepts and new materials

Time: Thursday 10:15–12:30

Location: EW 201

HL 71.1 Thu 10:15 EW 201

$YMnO_3$ - based MIS structure with a selective, capacitive photo-detecting properties — ●AGNIESZKA BOGUSZ^{1,2}, OM S. CHOUDHARY², ILONA SKORUPA¹, DANILO BÜRGER², ALEXANDER LAWERENZ³, OLIVER G. SCHMIDT^{2,4}, and HEIDEMARIE SCHMIDT² — ¹Institute Of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf — ²Department of Materials for Nano-electronics, Chemnitz University of Technology — ³CiS Forschungsinstitut für Mikrosensorik und Photovoltaik GmbH — ⁴Institute for Integrative Nanosciences, IFW-Dresden

This work investigates the $YMnO_3/Si_3N_4/p - Si$ structures in terms of novel, capacitance-based photo-detecting properties. Photocapacitance-voltage (C-V) characteristics of the $YMnO_3/Si_3N_4/p - Si$ structures have been determined at room temperature for a wide spectral range ($\lambda = 300-980$ nm). C-V characteristics indicate a charge trapping process which is used as the basis for novel approach to photodetectors. Our model discusses the immobilization of otherwise mobile charges in Si_3N_4 when the negative polarization charge of the multiferroic $YMnO_3$ [1] is at the $YMnO_3/Si_3N_4$ interface. The observed capacitance minima are well-defined by the direction of bias ramp. Voltages corresponding to these minima were further used as a reference point for a read out of capacitance in retention and optical selectivity tests. Results indicate that investigated structures exhibit a good photo-sensitivity of red light and the retention properties are non-volatile for one capacitance branch. [1]B.B. Van Aken et al. Nature Mater.3,164(2004)

HL 71.2 Thu 10:30 EW 201

Coulomb blockade in metal nanoparticle field-effect transistors — ●HAUKE LEHMANN, SVENJA WILLING, SANDRA MÖLLER, MIRJAM VOLKMANN, and CHRISTIAN KLINKE — Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, 20146 Hamburg, Germany

Metallic nanoparticles offer possibilities to build and improve basic electrical devices. The role of a semiconductor's bandgap is adopted by the Coulomb energy gap [1] due to the charging of the single particles' capacities. Thus, it is required to keep the nanoparticles individualized by tunnel barriers, while a merging of the particles would render them metallic again.

We synthesize monodisperse CoPt nanoparticles by colloidal chemistry [2]. Those particles are deposited via the Langmuir-Blodgett technique as highly-ordered homogeneous monolayers onto substrates with predefined gold electrodes. Additional structuring of the films yields stripes from individual nanoparticles. Such a defined channel can be controlled through a carefully adjusted gate voltage much more precisely compared to former experiments on whole nanoparticle films [3]. An insulating layer on top of the nanoparticles enables the application of a local top-gate electrode instead of using the global back gate. We find oscillations indicating the Coulomb blockade at temperatures of up to approximately 100 K.

[1] C. W. J. Beenakker, Phys. Rev. B **44**, 1646 (1991)[2] S. Lim et al., Nano Lett. **10**, 964 (2010)[3] Y. Cai et al., J. Appl. Phys. **114**, 034311 (2013)

HL 71.3 Thu 10:45 EW 201

Thermal rectification in asymmetric MoS₂ nanoribbons: a non-equilibrium molecular dynamics study — ●LEONARDO MEDRANO SANDONAS^{1,2}, RAFAEL GUTIERREZ¹, AREZOO DIANAT¹, and GIANAURELIO CUNIBERTI^{1,3,4} — ¹Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — ²Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — ³Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — ⁴Dresden Center for Computational Materials Science (DCCMS), TU Dresden, 01062 Dresden, Germany

We provide insights into the design and understanding of thermal rectifiers based on asymmetric MoS₂ nanoribbons. Non-equilibrium molecular dynamics (NEMD) simulations are used to study the influence of geometrical shapes on the thermal rectification. Our results point out that asymmetric MoS₂ nanoribbons can display considerable thermal rectification. Moreover, this rectifier effect increases with the asymmetry degree of the device but, as expected, it weakens with increasing lin-

ear dimensions. Among the geometrical shapes studied in the present work, T-shaped MoS₂ nanoribbons present the highest thermal rectification for each asymmetry degree. We also found that vibrational modes for frequencies greater than 380 cm⁻¹ are almost fully localized and spatially distributed on the edges of the asymmetric nanoribbons. Thus, similar to asymmetric and defective nanostructures made of a single material, we find that lateral confinement of the vibrational modes is a mechanism of thermal rectification in MoS₂ nanoribbons.

HL 71.4 Thu 11:00 EW 201

Full two-dimensional band-mapping of Ni-intercalated TiS₂ by momentum microscopy — ●SHIGEMASA SUGA^{1,2}, CHRISTIAN TUSCHE¹, YUICHIRO MATSUSHITA¹, MARTIN ELLGUTH¹, AKINORI IRIZAWA², and JÜRGEN KIRSCHNER^{1,3} — ¹Max-Planck-Institute of Microstructure Physics, Weinberg 2, Halle 06120, Germany — ²Institute of Scientific & Industrial Research, Osaka University, 8-1 Mihogaoka, Ibaraki, Osaka 567-0047, Japan — ³Institut für Physik, Martin-Luther-Universität, Halle, Germany

Atom intercalation into the van der Waals gap of a layered semiconductor TiS₂ can effectively modify its electronic properties in the bulk and surface. In order to probe the changes of its surface electronic structure on Ni intercalation, we have performed high-resolution and simultaneous two-dimensional photoelectron spectroscopy of Ni1/3TiS₂ by use of a momentum microscope. Full (k_x,k_y) band dispersions are revealed up to 2.0 Å⁻¹. Small electron Fermi surfaces (FSs) with noticeable dispersion observed near the M points in TiS₂ became much stronger in Ni1/3TiS₂, in which a very small hole FS pocket with clear dispersion is additionally observed near Γ point. Detailed new experimental results are compared with first principles theoretical band calculations. Differences between these materials are dominated by the contribution of the Ni 3d states of the surface Ni atoms positioned at the C3v site, being different from its D3d site beneath the surface. The use of a momentum microscope is demonstrated to be inevitable for clarifying detailed electronic structures of many solids under hot debates. M.E. acknowledges support by the BMBF (05K12EF1).

HL 71.5 Thu 11:15 EW 201

Determination of Optical and electronic structure properties studied for Sr[LiAl₃N₄]:Eu+2 as a next-generation LED-phosphor material. — ●SIKANDER AZAM¹, ROBIN NIKLAUS², WOLFGANG SCHNICK², and JAN MINAR^{1,2} — ¹New Technologies-Research Center, University of West Bohemia, Univerzitni 8, 306 14 Pilsen, Czech republic — ²Dept. of Chemistry, University of Munich, Germany

Recently, Sr[LiAl₃N₄]:Eu+2 has been shown to be a promising LED-phosphor material with a great potential for industrial application [1]. Using density functional theory (DFT) within the local density approximation (LDA), the generalized gradient approximation (GGA) and the modified Becke*Johnson (mBJ) form we investigated the structural, electronic and optical properties of Sr[LiAl₃N₄]:Eu+2. The total energy has been optimized as a function of the unit cell volume. All other parameters like the density of state (DOS), the band structure and the linear optical susceptibility are calculated for the relaxed structure applying the optimized lattice constant. We show that our calculated band structure agrees quantitatively very well with corresponding experimental data. It will be shown that for the calculation of optical properties, which are closely related to the corresponding electronic structure our results are an essential precondition. [1] P. Pust et al., Nature Mat. **13**, 891 (2014)

HL 71.6 Thu 11:30 EW 201

Coupled organic-inorganic nanostructures: Size dependent carrier transport in tetrathiafulvalenedicarboxylate capped PbS nanocrystals — ●ALEXANDER ANDRÉ^{1,2}, MAHDI SAMADI KHOSHKO^{1,2}, and MARCUS SCHEELE^{1,2} — ¹Institute of Physical and Theoretical Chemistry, University of Tübingen, Auf der Morgenstelle 18 72076 Tübingen — ²Center for Light-Matter Interactions, Sensors&Analytics (LISA+), Auf der Morgenstelle 15 72076 Tübingen

Both, inorganic semiconductor quantum dots (QD) and organic semiconductors (OSC), are emerging classes of materials for optoelectronic applications. QDs provide the possibility of size tailored optical and electronic properties all the while keeping sufficiently high charge car-

rier mobilities and diffusion lengths. OSCs however, offering high material purity and a large degree of ordering in thin films, have already been successfully implemented as transistors and light emitting devices. In our work we aim to combine these two material classes in order to get the best of both worlds. To that end we prepare coupled organic-inorganic nanostructures, so called COINs. Thin films of PbS nanocrystals, with different diameters, functionalized with tetrathiafulvalenedicarboxylate were fabricated via spin coating or superlattice self-assembly at a liquid-liquid interface. The morphology of the resulting samples was investigated with SEM, FT-IR and AFM. The conductivity and charge carrier mobility was measured using a field effect transistor setup. We can show the successful formation of highly ordered nanocrystal superlattices with charge carrier mobilities on the order of $10^{-4} \text{ cm}^2/V \cdot \text{s}$.

HL 71.7 Thu 11:45 EW 201

Nanointerfaces in InAs-Sn₂S₆ nanocrystal-ligand networks: atomistic and electronic structure from *first principles* —

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Semiconducting nanocomposites – consisting of nanocrystals (NCs) embedded in a host matrix – offer exciting prospects for solar energy conversion, light emission and electronic applications. Recent advances in wet chemical synthesis techniques allow for the synthesis of nanocrystals, their assembly into superlattices and embedding into a host matrix completely using only inexpensive solution processing. However, the atomistic details of the resulting nanocomposites are poorly understood, due to the complexity of the synthesis conditions and the unavailability of robust experimental techniques to probe nanointerfaces at the microscopic level. Here we present a density functional theory investigation of the interaction of Sn₂S₆ ligands with InAs NCs. Employing a grand canonical approach, we considered a multitude of structural features possibly realized at the NC-ligand interface, such as surface termination, reconstructions and passivation, substitution of subsurface atoms, ligand dissociation, NC core-shell formation and the adsorption of the ligands on NCs with different structures. This study provides guidance about the experimental conditions which lead to specific structural motifs and highlights the impact of structural details on the electronic properties of the composite.

HL 71.8 Thu 12:00 EW 201

Graphene 3D Electrodes for Energy Storage Applications —

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ment, TU München, Am Coulombwall 4, 85748 Garching

Due to its unique properties like high conductivity, chemical stability, and high surface to volume ratio, graphene meets the most essential requirements for fabricating electrodes with high electrical double layer capacitance for supercapacitor applications. Here we present the fabrication and characterization of graphene foam based electrodes for energy storage applications. Chemical vapor deposition (CVD) is used to grow graphene foam samples with nickel foam as a substrate. Different growth parameters are investigated in order to obtain stable three-dimensional structures as well as to achieve high graphene quality, which is confirmed by Raman spectroscopy. To decrease the equivalent series resistance and to have a highly inert contact, multilayer CVD graphene sheet was used to connect the foam to the current collector. Cyclic voltammetry, electrochemical impedance spectroscopy, and charge discharge measurements in various electrolytes are performed to assess the potential of these three-dimensional graphene electrodes for energy storage applications.

HL 71.9 Thu 12:15 EW 201

Conductive polymers on microporous graphene based electrodes for supercapacitor applications —

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Conductive polymers have been studied as pseudocapacitive electrode material owing to their high specific capacitance and high reaction rates. In order to increase the surface area and to have a efficient charge transfer, a highly conductive three-dimensional current collector is required for supercapacitors providing high power density. Graphene-based electrodes have a high specific area, a high conductivity and are chemical inert, which makes them a promising current collector material for supercapacitor applications.

Here we present three dimensional graphene electrodes coated with conductive polymers by electropolymerization and chemical polymerization for supercapacitor electrodes. As conductive polymers polyaniline, polypyrrole and polyphenylene were polymerized with different polymerization parameters like temperature and concentration. Polyaniline and polypyrrole are moderate conductive p-doped polymers, chemically stable in aqueous solutions and can be polymerized out of inexpensive precursors. Polyphenylene is a p- or n-doped conductive polymer which enables it to be operated in a high potential window in non-aqueous electrolytes. Their potential for supercapacitors is confirmed by cyclic voltammetry, electrochemical impedance spectroscopy and charge-discharge measurements.