

## CPP 12: Focus: Molecularly Functionalized Low-Dimensional Systems II - organized by Antonio Setaro, Carola Meyer, Aravind Vijayaraghavan and Matteo Mannini

See part I of the session for a synopsis.

Time: Monday 15:00–17:30

Location: C 130

**Topical Talk** CPP 12.1 Mon 15:00 C 130  
**Magnetoresistance in Single-Radical Molecular Junctions** — ●ELKE SCHEER — Department of Physics, University of Konstanz, 78457 Konstanz

We study the charge transport properties of single radical molecule junctions formed by a break junction technique at 4.2 K in magnetic field  $B$ . In this study, stable and neutral radical molecules based on an oligo(*p*-phenylene ethynylene) (OPE) backbone with a radical attached to its side (TEMPO-OPE) are contacted with freestanding and tunable gold (Au) electrodes. In perpendicular field we observe large positive magnetoresistance (MR) up to 287 % at 4T [1]. The average MR amplitude is one order of magnitude larger than that of the analogous non-radical OPE molecule. In parallel field a step-like negative MR occurs with the same amplitude on field scales of 2-3 T. The analysis of the MR, of current-voltage characteristics and of inelastic electron tunneling spectra reveal an effective reduction of the electronic coupling between the current-carrying frontier orbital and the metal electrodes with increasing  $B$ . Our findings thus provide a new physical approach for tuning the charge transport through radical molecules. [1] R. Hayakawa et al. *Nano Lett.* 16, 4960 (2016).

CPP 12.2 Mon 15:30 C 130  
**UHV deposition of pyrene on metal surfaces** — ●SEBASTIAN SCHLEICHER<sup>1</sup>, BOGDANA BORCA<sup>3</sup>, JEFF RAWSON<sup>2</sup>, FRANK MATTHES<sup>1</sup>, DANIEL E. BÜRGLER<sup>1</sup>, PAUL KÖGERLER<sup>2</sup>, and CLAUS M. SCHNEIDER<sup>1</sup> — <sup>1</sup>Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich — <sup>2</sup>Institute of Inorganic Chemistry, RWTH Aachen University — <sup>3</sup>National Institute of Materials Physics, Bucharest, Romania

Interfacial properties of organic adsorbates featuring aromatic  $\pi$ -orbitals on metal surfaces play an important role for organic electronics and spintronics. The deposition of single pyrene molecules with a size between ultimately small benzene and extended graphene on clean and reactive surfaces is challenging, since pyrene is a solid with a high vapor pressure. Hence, it cannot be evaporated from a Knudsen cell, nor dosed from the gas phase. Here, we present a sublimation procedure under UHV and image pyrene molecules on in-situ cleaned Au(111) and Fe/W(110) substrates by means of low temperature scanning tunneling microscopy (LT-STM) at 77 K. For the Au(111) surface, the molecule-surface interaction is weak such that the Au(111) herringbone reconstruction is not lifted and visible through the ordered molecular layer. Pyrene desorption self-limits growth to a monolayer due to the weak intermolecular bonding. The molecular arrangement of adsorbed pyrene on stronger interacting Fe films on W(110) sensitively depends on Fe thickness. Irregular configurations occur on the first Fe layer, while self-assembled ordered arrays form on the second, third and fourth Fe layer.

CPP 12.3 Mon 15:45 C 130  
**Spin-Dependent Electron Transmission Model for Chiral Molecules in Solid-State Nanodevices** — ●XU YANG — Zernike Institute for Advanced Materials, University of Groningen, Groningen, the Netherlands

Various experiments have indicated that electron-transfer in several chiral molecules is spin-dependent, a phenomenon known as the Chiral Induced Spin Selectivity effect. This holds promise for realizing spintronic nanodevices that do not contain ferromagnetic materials. However, due to the lack of theoretical understanding, it is not always clear to what extent the chiral molecules contribute to the spin-dependent signals. We aim to develop a spin-dependent electron transmission model that can quantitatively evaluate the role of chiral molecules in two-terminal, three-terminal and four-terminal transport measurements. As starting point, we use the universal symmetry of electrical conduction to explain the necessity of spin-flip electron reflection at chiral molecules. Based on this model, we propose new types of graphene- or carbon nanotube- based multi-terminal transport measurements that can separate the CISS effect from other spin-dependent signals. Our modeling provides a fundamental insight and an effective toolbox for understanding low-dimensional solid-state spintronic de-

vices functionalized with chiral molecules.

CPP 12.4 Mon 16:00 C 130  
**Electrical Characterization of Bis(terpyridine)ruthenium-Complex Functionalized Au-Nanoparticles in Heterometallic Nanoelectrode Gaps** — ●MAX MENNICKEN<sup>1</sup>, SOPHIA KNECHT<sup>2</sup>, CORINNA KAULEN<sup>2</sup>, ULRICH SIMON<sup>2</sup>, and SILVIA KARTHÄUSER<sup>1</sup> — <sup>1</sup>Peter Grünberg Institut (PGI-7), Forschungszentrum Jülich GmbH, Germany — <sup>2</sup>Institut für Anorganische Chemie (IAC), RWTH Aachen University, Germany

Following the concept of integrating molecular electronic devices into traditional CMOS circuitry, molecularly functionalized metal nanoparticles (NP) are employed. Especially complexes of ruthenium with chelating terpyridine ligands exhibit interesting properties. They can act as a switch of constant length, based on a redox mechanism, addressed by electrical or optical pulses. The application of 1,4-bis(2,2':6',2''-terpyridin-4'-yl)benzol (BTP) ligands as a linear linking moiety allows the formation of Ru-BTP diads, triads or even longer molecular wires. Here, we use 15 nm Au-NP functionalized with 4'-(4-mercaptophenyl)-2,2':6',2''-terpyridin (MPTP) and the corresponding (MPTP)<sub>2</sub>-ruthenium complex. We immobilized such Au-NP in between heterometallic nanoelectrode gaps consisting of AuPd and Pt. The resulting devices are characterized by SEM and transport measurements which are compared to estimations of the conductance through the respective molecules. Furthermore, the principle of growth of Ru-BTP based molecular wires is investigated by XPS measurements.

CPP 12.5 Mon 16:15 C 130  
**Impact of chemical treatment of diamond thin films on neuron growth** — BARBORA JAKUBCOVÁ<sup>1</sup>, JANA TURNOVÁ<sup>1</sup>, VÁCLAV PETRÁK<sup>1</sup>, PAVEL HUBÍK<sup>2</sup>, ANDREW TAYLOR<sup>2</sup>, and ●VLADIMÍRA PETRÁKOVÁ<sup>1,3</sup> — <sup>1</sup>Czech Technical University in Prague, Faculty of Biomedical Engineering, Kladno, Czech Republic — <sup>2</sup>Czech Academy of Sciences, Institute of Physics, Prague, Czech Republic — <sup>3</sup>Free University Berlin, Institute of Experimental Physics, Berlin, Germany

This work compares the impact of molecular functionalization and selected material properties of diamond thin films on the growth of neurons. The ability to form an efficient interface between material and neural cells is a crucial aspect of the construction of neuroelectrodes. Diamond thin films offer material characteristics that could greatly improve the performance of neuroelectrodes. The advantage of diamond is a large variety of material and surface properties. Such a variety of material characteristics can lead to various cellular responses. Here we compare growth and development of primary neural cells on diamond thin films of various morphology, conductivity, and doping with their treatment using several types of molecules commonly used to enhance adhesion and cell growth. We found that the variation of material properties of nanocrystalline diamond film does not have a major influence on the neuron growth but it can be to, some extent, influenced by the type of molecular coating, selection of polymer and its molecular weight. Our findings emphasize the importance of the correct molecular treatment over structural or morphological properties of diamond thin films as a material used to form an interface with primary neurons.

**15 min. break**

CPP 12.6 Mon 16:45 C 130  
**Nanowire field-effect transistor structures for the detection of cardiac biomarkers: troponin and C-reactive protein** — YURI KUTOVYI, IHOR ZADOROZHNYI, VOLODYMYR HANDZIUK, HANNA HLUKHOVA, NAZARI BOICHUK, and ●SVETLANA VITUSEVICH — Bioelectronics (ICS-8), Forschungszentrum Jülich, 52425 Jülich, Germany

Today high-speed operation is one of the key factors in the development of biosensors. Cardiac disease is one of the most critical diseases, requiring medical treatment within the first two hours of acute myocardial infarction (AMI). Cardiac troponin (cTn) remains the gold

standard in AMI diagnosis. cTn is released from the cardiac cell and its concentration typically increases after the onset of AMI. At the same time, C-reactive protein (CRP) can be used as a predictive biomarker to indicate the likelihood of AMI in the near future. In this presentation, we will discuss the design and fabrication of silicon nanowire field-effect transistor structures using CMOS-compatible technology as well as the results we obtained upon the detection of both proteins. We demonstrate that along with the threshold voltage shift measured as a function of charged molecule binding events, a number of new parameters due to single-trap phenomena can be used as the detection signal. Together with a gate coupling effect, the utilization of new parameters allows more sensitive monitoring of troponin and CRP behavior in addition to the realization of real-time compact devices for point-of-care applications. Authors gratefully acknowledge the Innovation Award RWTH transparent 2016.

CPP 12.7 Mon 17:00 C 130

**Ultrasensitive and selective detection of biomarkers with bio-functionalized graphene field effect transistors** — •DAVID KAISER<sup>1</sup>, NIKOLAUS MEYERBROEKER<sup>2</sup>, WERNER PURSCHKE<sup>3</sup>, ANDREAS WINTER<sup>1</sup>, CHRISTOF NEUMANN<sup>1</sup>, THOMAS WEIMANN<sup>4</sup>, ALBERT SCHNIEDERS<sup>2</sup>, AXEL VATER<sup>3</sup>, and ANDREY TURCHANIN<sup>1</sup> — <sup>1</sup>Institute for Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — <sup>2</sup>CNM Technologies GmbH, 33607 Bielefeld, Germany — <sup>3</sup>APTARION biotech AG, 10589 Berlin, Germany — <sup>4</sup>Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany

Due to the unique properties of graphene, graphene-based field effect transistors (GrFETs) are promising electronic devices for sensing of biological molecules. In this contribution, we present a concept of novel hybrid BioGrFETs for selective and ultrasensitive detection of biomarkers based on graphene functionalized non-covalently with L-

aptamers via a molecular carbon nanomembrane (CNM). We demonstrate that the engineered BioGrFETs have up to 3 orders of magnitude dynamic range and reach a sensitivity limit down to 1 pM for selected biomarkers. We characterize the subsequent fabrication steps on the nanoscale by surface science and biochemical techniques and describe the BioGrFETs transfer characteristics by an electrochemical model of the heterostructure interface.

CPP 12.8 Mon 17:15 C 130

**Proton Transport Through 2D Membranes** — •YUN AN<sup>1</sup>, AGNIESZKA KUC<sup>1</sup>, PETKO PETKOV<sup>2</sup>, and THOMAS HEINE<sup>1</sup> — <sup>1</sup>Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Leipzig, Germany — <sup>2</sup>Faculty of Chemistry and Pharmacy, University of Sofia, 1164 Sofia, 1 James Bourchier Blvd., Bulgaria

Conventional membranes have been used for sieving atomic and molecular species, however, they have no subatomic selectivity. Recently, two dimensional (2D) crystals, such as graphene and hexagonal boron nitride (hBN), have been shown to be good candidates for hydrogen isotope sieving. Nevertheless, the mechanism of such a process has not been reported so far. Therefore, to understand the proton transport through 2D membranes is of great importance. Aiming at this, we have studied theoretically what happens with protons when introduced between 2D layers. Density functional theory (DFT) together with well-tempered metadynamics simulations was employed to study dynamics of proton transfer in between the layers. Our studies reveal that lattice vibrations are crucial for understanding the phonon calculations. While they can be well described using Born-Oppenheimer DFT based metadynamics simulations, static transition state calculations at the same level of theory lead to very high barriers that are unsuitable to describe the experimental observations.