

## TT 24: Molecular Electronics and Photonics

Time: Tuesday 9:30–12:15

Location: H22

TT 24.1 Tue 9:30 H22

**Heat transport through single-atom and single-molecule junctions** — ●FABIAN PAULY — Okinawa Institute of Science and Technology Graduate University, Okinawa, Japan

In this presentation, I will discuss our present theoretical understanding of heat transport at the atomic scale. Starting from results of a collaboration with experimentalists [1], I will elucidate the importance of phonons for the thermal conductance of atomic-size contacts made of different metals [2] and will examine the validity of the Wiedemann-Franz law, which relates the electrical and the thermal conductance. Next, I will present a newly developed procedure to determine transmission eigenchannels for coherent phonon transport in nanoscale devices using the framework of nonequilibrium Green's functions [3]. To illustrate its value, I will study phonon eigenchannels in various systems ranging from metallic atomic-size contacts to different single-molecule junctions.

[1] L. Cui et al., *Science* 355, 1192 (2017)

[2] J. C. Klöckner et al., *Phys. Rev. B* 96, 205405 (2017)

[3] J. C. Klöckner et al., *Phys. Rev. B* 97, 155432 (2018)

TT 24.2 Tue 9:45 H22

**Large Conductance Variations in a Mechanosensitive Single-Molecule Junction** — ●MAXIM SKRIPNIK<sup>1,2</sup>, DAVIDE STEFANI<sup>3</sup>, KEVIN J. WEILAND<sup>4</sup>, CHUNWEI HSU<sup>3</sup>, MICKAEL L. PERRIN<sup>3,5</sup>, MARCEL MAYOR<sup>4,6,7</sup>, HERRE S. J. VAN DER ZANT<sup>3</sup>, and FABIAN PAULY<sup>1,2</sup> — <sup>1</sup>Okinawa Institute of Science and Technology, Japan — <sup>2</sup>University of Konstanz, Germany — <sup>3</sup>Delft University of Technology, The Netherlands — <sup>4</sup>University of Basel, Switzerland — <sup>5</sup>Swiss Federal Laboratories for Materials Science and Technology, Switzerland — <sup>6</sup>Karlsruhe Institute of Technology, Germany — <sup>7</sup>Sun Yat-Sen University, China

Using quantum-chemistry calculations we show that the conductance of a spring-like molecule can be mechanically controlled by several orders of magnitude by compressing or elongating it. [1] The calculations indicate that the large conductance variations are the result of a destructive quantum interference between the frontier orbitals. Furthermore, oscillations in the conductance occur when the stress built up in the molecule is high enough to allow the anchoring groups to move along the surface in a stick-slip-like fashion. Theoretical results are very well supported by break-junction measurements which demonstrate that the large conductance variations are also present at room temperature. This may open the door for applications in, e.g., a nanoscale mechanosensitive sensing device that does not rely on cryogenic cooling.

[1] D. Stefani et al., *Nano Lett.* 18, 5981 (2018).

TT 24.3 Tue 10:00 H22

**High Magnetoresistance and Kondo Resonance in Radical Molecular Junctions** — ●GAUTAM MITRA<sup>1</sup>, DAVID WEBER<sup>1</sup>, JONATHAN LOW<sup>2</sup>, SUJUN WEI<sup>2</sup>, KAROL FRANCISCO<sup>2</sup>, LUIS CAMPOS<sup>2</sup>, and ELKE SCHEER<sup>1</sup> — <sup>1</sup>Department of Physics, University of Konstanz, Germany — <sup>2</sup>Department of Chemistry, Columbia University, New York, United States

The presence of an unpaired electron in organic radical molecules gives rise to intrinsic magnetic properties when coupled to nonmagnetic electrodes. In the present study, we report on the magnetic behavior of polychlorotriphenylmethyl radical molecule [1] junctions using the mechanically controlled break junction technique. The transport measurements were carried out at low temperatures down to 1.5K. We have observed very high positive and negative magnetoresistance up to 140% for a magnetic field of 6T applied perpendicular to the current direction. Alongside, we also observe significant zero bias anomalies corresponding to Kondo temperatures around 9K, originates from a spin flipping Kondo mediated transport channel as observed for a similar molecule contacted by rigid electrodes before [2]. Meanwhile the exact origin of magnetoresistance behavior from this molecule is still unknown and open for further investigation. By changing the inter-electrode spacing, we follow the development of the Kondo resonance and magnetoresistance which further opens up the relation between coupling of electrodes with molecule.

[1] Armet, O. et.al. *J. Phys. Chem.* 1987, 91, 5608-5616

[2] Frisenda, R. et.al. *Nano Lett.* 2015, 15, 3109-3114

TT 24.4 Tue 10:15 H22

**Conductance switching by CO adsorption in Ag point contacts** — ATASI CHATTERJEE<sup>1</sup>, FREDERIK EDLER<sup>1,2</sup>, CHRISTOPH TEGENKAMP<sup>1,2</sup>, and ●HERBERT PFNÜR<sup>1</sup> — <sup>1</sup>Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — <sup>2</sup>Institut für Physik, TU Chemnitz, Germany

We demonstrate that atomic point contacts can be generated at well-defined locations with extreme reliability in ultra-thin (5 nm) and ultra-small (minimum width 16 nm) Ag nanostructures, grown on hydrogen terminated low-doped Si (100) samples using the process of electro-migration at 100K inside a 4-tip SEM/STM UHV chamber. Single contacts were always obtained once the smallest constriction of the structures was below the average grain size of the Ag films and competing thermal migration was suppressed. Conductance histograms exhibit characteristic conductance values that were assigned to the different metastable configurations prior to atomic point contact formation. In-situ chemisorption of CO strongly altered the conductance from  $0.9G_0 < \sigma < 1.3G_0$  to a stable value close to  $0.1G_0$ , suggesting adsorption of single CO molecules within the contact. In the presence of CO, current versus voltage curves showed a slightly rectifying behavior indicating preferential binding of CO to one side of the electrode. Furthermore, time resolved current measurements at 100K demonstrate voltage-induced bi-stable conductance at 0.08 and 0.14  $G_0$  with stability of the 0.14  $G_0$  value below 0.1 V and of the lower conductance above 0.25 V, whereas at intermediate voltages switching between these values was observed.

TT 24.5 Tue 10:30 H22

**Molecular junctions and molecular motors: Inclusion of electron-electron interactions in the electronic friction** — ●MIROSLAV HOPJAN<sup>1,2</sup>, GIANLUCA STEFANUCCI<sup>3,4</sup>, ENRICO PERFETTO<sup>3,5</sup>, and CLAUDIO VERDOZZI<sup>2</sup> — <sup>1</sup>current: Condensed Matter Theory, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — <sup>2</sup>Department of Physics, Lund University, S-22100 Lund, Sweden — <sup>3</sup>Dipartimento di Fisica, Università di Roma Tor Vergata, Via della Ricerca Scientifica 1, I-00133 Rome, Italy — <sup>4</sup>INFN, Sezione di Roma Tor Vergata, Via della Ricerca Scientifica 1, I-00133 Roma, Italy — <sup>5</sup>CNR-ISM, Division of Ultrafast Processes in Materials (FLASHit), Area della Ricerca di Roma 1, Via Salaria Km 29.3, I-00016 Monterotondo Scalo, Italy

A semi-classical Ehrenfest (or Langevin) dynamics of current-induced forces in molecular junctions with electron-electron interactions will be presented. For the regime of slow nuclear dynamics we derive a general formula of the Markovian electronic friction, described within the one-particle non-equilibrium Green's function formalism. The proposed framework is approximations-free but at the same time it enables the direct use of many-body perturbation theory to include the interactions, thus it is suitable for practical calculations. Using a paradigmatic model and by benchmarking to non-Markovian dynamics we demonstrate the validity and numerical efficiency of the proposed scheme. We observe that the interactions can dramatically reduce the possibility of a negative friction coefficient, thus the self-sustainable current induced motion (i.e. molecular motor) can be suppressed by the interactions.

15 min. break.

TT 24.6 Tue 11:00 H22

**Electron Transport through single Mn-salen molecule: Theoretical Study** — ●LOKAMANI LOKAMANI<sup>1</sup>, FILIP KILIBARDA<sup>1,2</sup>, TORSTEN SENDLER<sup>1</sup>, PETER ZAHN<sup>1</sup>, MICHAEL MORTENSEN<sup>3</sup>, KURT VESTERAGER GOTHELF<sup>3</sup>, ARTUR ERBE<sup>1,2</sup>, and SIBYLLE GEMMING<sup>1,4</sup> — <sup>1</sup>Institute of Ion Beam Physics and Materials Research, HZDR, 01328 Dresden, Germany — <sup>2</sup>Dept. of Physics, Universität Konstanz, 78457 Konstanz, Germany — <sup>3</sup>iNANO and Dept. of Chemistry, University Aarhus, 8000 Aarhus, Denmark — <sup>4</sup>Institute of Physics, Technische Universität, 09107 Chemnitz, Germany

Metal-salen complexes, formed by the coordination of a metal cation and a N,N'-bis(salicylidene)ethylenediamine-based ligand, are promising candidates for molecular electronics, because of possible modulations of transport channels using different metal cations. One such candidate is Mn-salen complex.

Here, we first explore the electronic structure of single molecules using wave function (MS-CASSCF) and density-functional (DFT+U) methods. We then employ the non-equilibrium Green's function (NEGF) technique to study electron transport through single molecules attached to gold electrodes under finite bias. We explore various docking configurations for the single molecule between the gold electrodes.

A comparison with experimental coupling constants and energy levels, obtained using mechanically controllable break junction (MCBJ) technique is also presented.

TT 24.7 Tue 11:15 H22

**Electron Transport through single Mn-salen molecule: Experimental Study** — ●FILIP KILIBARDA<sup>1,4</sup>, LOKAMANI LOKAMANI<sup>1</sup>, TORSTEN SENDLER<sup>1</sup>, MICHAEL MORTENSEN<sup>2</sup>, KURT GOTHELF<sup>2</sup>, PETER ZAHN<sup>1</sup>, SIBYLLE GEMMING<sup>1,3</sup>, and ARTUR ERBE<sup>1,4</sup> — <sup>1</sup>Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — <sup>2</sup>iNANO and Dept. of Chemistry, University Aarhus, 8000 Aarhus, Denmark — <sup>3</sup>Institute of Physics, Technische Universität, 09107 Chemnitz, Germany — <sup>4</sup>Dept. of Physics, Universität Konstanz, 78457 Konstanz, Germany

Molecular electronics offers new ways for scaling down nanoelectronic components and making their production and operation more energy efficient. Our research focuses on classifying different molecules with the help of Mechanically Controlled Break Junction (MCBJ).

Here, we perform measurements on salen molecule and metal-salen complexes in liquid environments. They are explored as candidates for “chemical doping”, because they provide the possibility to fine-tune electrical properties by using different molecular inclusions. We measure both constant voltage vs. distance and *IV* characteristic of our metal-molecule-metal junctions.

Measurements are then fitted to a theoretical model, which takes the contribution of a single molecular level into account. From this model the energy of the molecular level and the coupling to the electrodes can be extracted and compared to first principles calculations.

TT 24.8 Tue 11:30 H22

**Proximity effects of a STM tip on the magnetic properties of Fe-porphyrin on Au(111)** — LAËTITIA FARINACCI<sup>2</sup>, ●SUMANTA BHANDARY<sup>1</sup>, REECHT GAEL<sup>2</sup>, SILKE BIERMANN<sup>1</sup>, and KATHARINA FRANKE<sup>2</sup> — <sup>1</sup>Centre de Physique Théorique, Ecole Polytechnique, 91128 Palaiseau, France — <sup>2</sup>Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

We have investigated the adsorption of Fe-porphyrin (FeP) molecules on a Au (111) surface. By means of Scanning Tunnelling Microscopy (STM), we show that the FeP molecules are preferentially adsorbed on the fcc and hcp areas of the surface. Density functional calculations suggest the top-site to be the most stable adsorption site for FeP monomers. The electronic and magnetic features of adsorbed molecules depend largely on the hybridization with the Au surface as well as with the STM tip, and can only be modeled by taking into account the large effective Coulomb interactions, crystal field and spin-orbit coupling at the Fe centre. The tip-molecule, as well as surface-molecule hybridizations are tuned by approaching the STM tip, revealing changes in the magnetic fingerprints of molecules in the STM spectra. Based on density functional theory and many-body theory, we show that the ground state electronic configuration is changed as the tip approaches

the molecule, changing the magnetic anisotropy and hence the STM spectra, while the spin state remains unchanged.

TT 24.9 Tue 11:45 H22

**On surface formation of 1D polyferrocenylene chains on metal surfaces with unique structural and electronic properties** — ●VIJAI MEENA SANTHINI<sup>1</sup>, OLEKSANDR STETSOVYCH<sup>1</sup>, MARTIN ONDRACEK<sup>1</sup>, MARTIN SVEC<sup>1</sup>, JESUS MENDIETA<sup>1</sup>, BRUNO DE LA TORRE<sup>1,3</sup>, IRENA G.STARA<sup>2</sup>, IVO STARY<sup>2</sup>, RADEK ZBORIL<sup>3</sup>, and PAVEL JELENIK<sup>1</sup> — <sup>1</sup>Institute of Physics, Czech Academy of Sciences, Praha, Czech Republic — <sup>2</sup>Institute of Chemistry and Biochemistry, Czech Academy of Sciences, Praha, Czech Republic — <sup>3</sup>Regional Centre of Advanced Materials and Technologies, Olomouc, Czech Republic

We present a novel way of generation of long flexible 1D polyferrocenylene chains on metal surface with lengths up to 50 nm, representing the longest homo-coupled polyferrocenylene up to our knowledge. We employ on surface Ullman coupling polymerization of 1,1'-diiodobiferrocene molecules, deposited at room temperature under ultra-high vacuum conditions. The product are analysed using the low temperature scanning tunnelling microscope/atomic force microscopy (LT-STM/AFM). We observe two distinct 2D well-ordered polymer islands after annealing, with different electronic structure, due to the different packing of 1D molecular nanowires within the islands. We identified the internal molecular arrangement of island with help of high-resolution STM/AFM imaging with functionalized tips. We also succeeded in pulling out the 1D PFC chains from the islands to form free-standing 1D chains. We have identified a transition in the electronic behaviour, from semiconducting polymer 2D islands to metallic 1D chains using scanning tunneling spectroscopy.

TT 24.10 Tue 12:00 H22

**Tunable quantum interference in ferrocene-based molecular junctions** — ●MARÍA CAMARASA-GÓMEZ<sup>1</sup>, DANIEL HERNANGÓMEZ-PÉREZ<sup>1</sup>, MICHAEL S. INKPEN<sup>2</sup>, GIACOMO LOVAT<sup>2</sup>, LATHA VENKATARAMAN<sup>2</sup>, and FERDINAND EVERS<sup>1</sup> — <sup>1</sup>Institute of Theoretical Physics, Regensburg University, D-93053 Regensburg (Germany) — <sup>2</sup>Department of Applied Physics and Chemistry, Columbia University, New York, NY 10027 (USA)

Ferrocene is a well-known organo-metallic compound comprising a single iron atom ‘sandwiched’ between two cyclopentadiene rings. However, not many of the transport properties of an isolated ferrocene have actually been measured [1] or calculated [2, 3]. We here present a computational study of ferrocene and ferrocene moieties employing density functional theory-based quantum transport calculations inspired by recent experimental scanning-transport break junction measurements. Our results suggest that ferrocene-derived species exhibit interesting quantum interference properties: we find Fano-type resonances due to the localized d-states of the ferrocene metal, as well as mechanically-tunable anti-resonances. The latter can change dramatically the conductance at the Fermi level by orders of magnitude in a relatively controlled manner. Our numerical findings are rationalized by an effective three-level tight-binding model which explains the key role of the symmetries of frontier molecular orbitals in the position and shape of the quantum interference.

[1] S. A. Getty, et al., Phys. Rev. B 71, 241401 (2005)

[2] K. Kanthasamy et al., Small 12, 4849 (2016)

[3] X. Zhao, et al., Phys. Rev. B 96, 085421 (2017)