

TT 74: Molecular Electronics and Photonics

Time: Wednesday 16:00–18:30

Location: H 3005

TT 74.1 Wed 16:00 H 3005

Unimolecular NAND logic gate with input by single Au atoms — ●DMITRY SKIDIN¹, JUSTUS KRÜGER¹, FRANK EISENHUT¹, ANDRE GOURDON², GIANAURELIO CUNIBERTI^{1,3}, CHRISTIAN JOACHIM², and FRANCESCA MORESCO¹ — ¹Institute for Materials Science, Max Bergmann Center of Biomaterials, and Center for Advancing Electronics Dresden, TU Dresden, 01069 Dresden, Germany — ²CEMES, CNRS, 29 rue J. Marvig, 31055 Toulouse Cedex, France — ³Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01069 Dresden, Germany

Design and fabrication of nanoscale functional electronic units remains a main task of molecular electronics. In this study, we combine on-surface synthesis approach with STM manipulation techniques to create a unimolecular NAND logic gate. For this purpose, we use asymmetric starphene, which has a characteristic Y-shape, but with the two branches being one phenyl ring longer than the other one. It is obtained by surface-assisted cyclodehydrogenation on Au(111). As predicted by theoretical calculations, local perturbations of the longer branches (which serve as an input) lead to the electronic changes on the shorter branch (output). The perturbations are provided by the interaction with the single Au atoms created on the surface. Scanning tunneling spectroscopy signal showing the position of the molecular resonance is used as an output. Thus, by carefully bringing the single Au atoms into interaction with the molecule, we induce the shifts of the resonant state in a way that replicates the Boolean truth table of a NAND logic gate.

TT 74.2 Wed 16:15 H 3005

Time-dependent framework for energy and charge currents in nanoscale systems — ●THOMAS LEHMANN¹, ALEXANDER CROY^{1,2}, RAFAEL GUTIÉRREZ^{1,2}, and GIANAURELIO CUNIBERTI^{1,2,3} — ¹Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — ²Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden, Germany — ³Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany

The calculation of time-dependent charge and energy currents in nanoscale systems is a challenging task. Nevertheless it is crucial for gaining a deep understanding of the relevant processes at the nanoscale. We extend the auxiliary-mode approach for time-dependent charge transport to allow for the calculation of energy and heat currents for arbitrary time-dependencies. We apply the approach to illustrative examples, demonstrating its usefulness for a wide-range of problems, such as thermoelectric effects in driven systems.

TT 74.3 Wed 16:30 H 3005

Current-induced bond rupture in molecular junctions — ●ANDRÉ ERPENBECK¹, URI PESKIN², and MICHAEL THOSS^{1,3} — ¹Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, 91058 Erlangen, Germany — ²Schulich Faculty of Chemistry & Lise Meitner Center for Computational Quantum Chemistry, Technion-Israel Institute of Technology, Haifa 32000, Israel — ³Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Strasse 3, 79104 Freiburg, Germany

Coupling between electronic and vibrational degrees of freedom in molecular junctions is an important mechanism, which influences the conductance properties. It also causes current-induced vibrational excitation, which may trigger bond rupture and is thus crucial in the context of the stability of molecular junctions. In this contribution, we study current-induced dissociation in molecular junctions based on representative models. To this end, we apply the hierarchical quantum master equation approach to the electronic transport problem. For the treatment of the nuclear degree of freedom, modeled with dissociative potentials, two different levels of theory are considered, (i) a quantum-classical description within the Ehrenfest approach and (ii) a fully quantum mechanical treatment using a discrete variable representation. Comparing the two approaches, we identify different processes leading to current-induced dissociation such as transient population of anti-bonding states by tunneling electrons or current-induced heating of the nuclear motion. The significance of the processes and their dependence on different model parameters is discussed in some detail.

TT 74.4 Wed 16:45 H 3005

Switching the conductance of molecular junctions by proton transfer — ●DOMINIK WECKBECKER¹, PEDRO B. COTO¹, and MICHAEL THOSS^{1,2} — ¹FAU Erlangen-Nürnberg, Institut für Theoretische Physik, Staudtstrasse 7/B2, 91058 Erlangen, Germany — ²Universität Freiburg, Physikalisches Institut, Hermann-Herder-Str. 3, 79104 Freiburg

While most experiments on single-molecule junctions have employed metal electrodes, recent works demonstrate that graphene has a number of advantages over metallic leads [1-2]. In this contribution, we investigate charge transport in graphene-molecule junctions employing a theoretical approach that combines first-principles electronic structure methods with nonequilibrium Green's function transport theory [3]. Specifically, we consider zigzag and armchair terminated graphene leads with covalently bonded molecular bridges. We analyze the possibility to use a proton transfer reaction as novel mechanism for switching the conductance of a molecular junction. Our simulations demonstrate that an intramolecular proton transfer can change the conductance of the graphene-molecule junction significantly [4]. While a proton transfer parallel to the transport direction could be used to realize a molecular switch or diode, a junction with a perpendicular proton transfer can resemble a transistor.

[1] K. Ullmann et al., *Nano Lett.* 15, 3512 (2015)[2] C. Jia et al., *Science* 352, 1443 (2016)[3] M. Brandbyge et al., *Phys. Rev. B* 65, 165401 (2002)[4] D. Weckbecker et al., *Nano Lett.* 17, 3341 (2017)

TT 74.5 Wed 17:00 H 3005

Characteristic excitations in conduction through Ag-CO molecular junctions — ●ATASI CHATTERJEE¹, JAN PHILIPP STÖCKMANN¹, CHRISTOPH TEGENKAMP^{1,2}, and HERBERT PFNÜR¹ — ¹Leibniz Universität Hannover, Institut für Festkörperphysik, 30167, Hannover, Germany — ²Technische Universität Chemnitz, Institut für Physik, 09126, Chemnitz, Germany

Ag metallic nano-electrodes with an initial centre width of approximately 20 nm were fabricated using a combination of e-beam lithography (EBL) and focused ion beam (FIB) milling. These structures were thinned by electromigration (EM) to generate atomic point contacts. With the help of a 4-tip SEM / STM setup, the visualization of the structural changes as well as conductance measurements were performed at the same time. Conductance histograms exhibit characteristic signatures of atomic point contacts. Conductance of these point contacts was strongly altered by adsorbed CO, which was deposited in-situ after opening the contact. Sub-G₀ plateaus were observed as first signatures of the metal molecule interaction. I-V measurements were performed at sub-G₀ values when the conductance was stable for at least 15 mins. The I-V curves are asymmetric with a slightly rectifying behavior for negative voltages. This asymmetry can be attributed to the fact that CO molecule binds preferably to one side of the metallic electrode. From the characteristic changes of slope, resonance features, and change of noise levels at different voltages in the IV measurements, we explain the properties of these Ag-CO molecular junctions.

15 min. break.

TT 74.6 Wed 17:30 H 3005

Tension related vibrational frequency shifts in helicene molecules — ●YUXIANG GONG¹, CHAO JING¹, PETER HASCH¹, JOACHIM REICHERT¹, IVO STARÝ², and JOHANNES BARTH¹ — ¹Physik Department, Technische Universität München, James-Frank-Str. 1, 85748 Garching, Germany — ²Institute of Organic Chemistry and Biochemistry ASCR, v.v.i. Flemingovo nám. 2, CZ-166 10 Prague 6, Czech Republic

The investigation of electronic properties of organic molecules is a fundamental aspect in the field of molecular electronics. Molecular transistors, switches and amplifiers have been demonstrated. In this work, a single-molecule junction spectroscopy (MJS) technique is applied to detect the current-voltage characteristics and vibrational properties of 1,7-dithiol-7-helicene molecules simultaneously. The single-molecule junction can be established by approaching the substrate to a gold covered tetrahedral scanning near-field tip, which is monitored via Raman spectroscopy. Afterwards, the substrate is carefully retracted,

stretching the molecule. At each step, a Raman spectrum is acquired. One distinct vibrational mode is analyzed, and reveals a systematic red shift corresponding to the applied strain in the single-molecule junction. The experimental results are complemented and explained by DFT simulations which take the electrodes into consideration.

TT 74.7 Wed 17:45 H 3005

Quantum Transport Properties of Silane Molecular Wires — •MARÍA CAMARASA-GÓMEZ¹, HAIXING LI², TIMOTHY A. SU², DANIEL HERNANGÓMEZ-PÉREZ¹, LATHA VENKATARAMAN², and FERDINAND EVERS¹ — ¹Institute of Theoretical Physics, University of Regensburg, D-93040 Regensburg (Germany) — ²Department of Applied Physics and Chemistry, Columbia University, New York, NY 10027 (USA)

In single-molecule junction experiments the conduction of silane wires attached to Au and Ag electrodes has been measured for thiol- and amine-based anchoring groups [1]. The experimental results show that amine-terminated molecules present lower conductance when attached to Ag than Au. The result is in agreement with expectations based on the trends in the metal work function. Surprisingly, the trend is reversed with thiol-linkers.

We present a theoretical analysis employing transport calculations based on the density functional theory that explains this result. Our study shows how the chemical nature of the bonds between anchor groups and metal electrodes can influence the conductance trends. We conclude that the influence of anchor groups can be large and sometimes even dominating over a work function related level mismatch.

[1]H. Li, T. A. Su, M. Camarasa-Gómez et. al., *Angew. Chem. Int. Ed.* 56, 14145 (2017)

TT 74.8 Wed 18:00 H 3005

Quantum Transport Properties of Polymethine and Polyene Molecular Wires — •DANIEL HERNANGÓMEZ-PÉREZ¹, SUMAN GUNASEKARAN², IRYNA DAVYDENKO³, SETH MARDER³, FERDINAND EVERS¹, and LATHA VENKATARAMAN^{2,4} — ¹Institute of Theoretical Physics, University of Regensburg, D-93050 Regensburg, Germany — ²Department of Chemistry, Columbia University, New York, New

York 10027, United States — ³School of Chemistry and Biochemistry and Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, Georgia 30332-0400, United States — ⁴Department of Applied Physics and Applied Mathematics, Columbia University, New York, New York 10027, United States

We report recent results on quantum transport properties of polymethine and polyene molecular wires. These wires represent a class of linear conjugated molecules which can be understood in the context of the topological Su-Schrieffer-Heeger model. Here, we present conductance measurements in polymethine dye junctions obtained with the scanning tunneling microscope break junction technique. Supported by tight-binding and ab-initio calculations, we argue that the lack of exponential decay in the conductance trends with the system length is due to the small bond-length alternation present in the polymethine wires. We finally discuss conditions for the observation of topological modes in quantum transport experiments.

TT 74.9 Wed 18:15 H 3005

Rotational dynamics of model molecular gears: non-equilibrium Green's function approach — •HUANG-HSIANG LIN^{1,2}, ALEXANDER CROY¹, RAFAEL GUTIÉRREZ¹, and GIANAURELIO CUNIBERTI^{1,3,4} — ¹Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01069 Dresden, Germany — ²Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — ³Dresden Center for Computational Materials Science, TU Dresden, 01062 Dresden, Germany — ⁴Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany

The possibility of creating nanoscale molecular gears has opened novel routes to implement true molecule-based mechanical analogs. Here, we investigate, within a model Hamiltonian approach, the rotational dynamics of a molecular gear. For this, we combine Langevin dynamics and non-equilibrium Green's functions to compute current-induced torque and damping, which allows it to study the influence of the electronic system on the rotational dynamics. Our model provides the rotational analog of the Anderson-Holstein Hamiltonian. To demonstrate the typical behavior of the gear, we present analytical and numerical calculations.