CPP 21: Transport: Molecular Electronics (joint session TT/CPP/HL/MA)

Time: Wednesday 9:30–12:45 Location: H2

CPP 21.1 Wed 9:30 H2

Inelastic scattering effects and electronic shot noise — •Amin Karimi, Markus Herz, and Elke Scheer — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

The study of shot noise for junctions formed by single molecules offers interesting new information that cannot be easily obtained by other means. At low bias it allows determining the transmission probability and the number of current carrying conductance channels [1]. We investigate the effects of phonon scattering on the electronic current noise through nano junctions with mechanically controllable break junction (MCBJ). Equivalent measurements have recently been reported to be able to reveal inelastic transport contributions to the current through gold atomic contacts [2]. We developed a new and versatile measurement system enabling measurements of the noise in a rather broad range of conductance values from 0.01 G_0 to 1 G_0 without the necessity of double wiring. First results on gold atomic contacts and benzendithiol will be presented.

[1] D. Djukic and J. M. van Ruitenbeek, Nano Lett. 6, 789-793 (2006)
[2] M. Kumar, R. Avriller and J. M. van Ruitenbeek, Phys. Rev. Lett. 108, 146602 (2012)

CPP 21.2 Wed 9:45 H2

Electrical Characterization of Single Molecules via MCBJ — •Matthias Wieser[1], Torsten Sendler[1], Shou-Peng Liu[2], Samuel Weisbrod[2], Zhuo Tang[2], Andreas Marx[2], Jannic Wolf[2], Elke Scheer[2], Francesca Moresco[3], Grebing Jochen[1], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., D-01328 Dresden — [2]Universität Konstanz, D-78457 Konstanz — [3]Max Bergmann Center of Biomaterials, D-01069 Dresden

For future molecular electronics applications the detailed knowledge about the electrical transport properties of single molecules is very important. To achieve this goal we are using the mechanical controllable break junction technique in liquid environments in combination with insulating substrates. We characterize the electrical conductance and I-V characteristics of single molecules which consist of three phenyl rings connected by triple carbon bonds with two oxygen sidegroups binding to the central ring. The I-V characteristics are further investigated by creating 2D histograms for hundreds of I-V curves and by fitting a single level model which provides us the metal-molecule junction coupling constants and the molecular energy level.

CPP 21.3 Wed 10:00 H2

Charge transmission through a molecular junction driven by a time–dependent voltage — •Yaroslav Zelinskyy[1,2], Yoram Selzer[3], and Volkhard May[1] — [1]Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, D-12489 Berlin, Germany — [2]Bogolubov Institute for Theoretical Physics, National Academy of Science of Ukraine, 14-b Metrologichna str., UA-03683, Kiev, Ukraine — [3]School of Chemistry, Tel Aviv University, Ramat Aviv, 69978 Tel Aviv, Israel

Time-dependent electron transport through a molecular junction driven by voltage pulses with a duration even in the sub-ps region is investigated theoretically. The transient behavior of the current is analyzed in focusing on the sequential transport regime and in utilizing a density matrix approach. As a quantity detectable in the experiment the averaged dc-current resulting from a sequence of voltage pulses is also calculated. The obtained data are analyzed with respect to their dependence on the voltage pulse shape, the magnitude and asymmetry of the lead-molecule coupling, and the mechanism and strength of intramolecular relaxation. All the findings are confronted with recent computations on transient currents due to optical excitation of the junction [1,2].

[1] L. Wang and V. May, Phys.Chem.Chem.Phys. 13, 8755 (2011)
[2] Y. Zelinskyy and V. May, Nano Lett. 12, 446 (2012)).

CPP 21.4 Wed 10:15 H2

Surface Plasmon Enhanced Electroluminescence of a Molecular Junction — •Yuan Zhang[1,2], Yaroslav Zhelinskyy[1], and Volkhard May[1] — [1]Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, D-12489 Berlin, Germany — [2]University of Science and Technology Beijing, XueYuan Road 30, 100083 Beijing, P. R. China

There are some first experiments indicating surface plasmon enhanced emission of a molecular junction. We present a coherent theory for this phenomenon, which is based on our previous work on molecule metal nanoparticle complexes [1,2,3,4]. Ultilizing a density matrix description our theory accounts for electron transfer in junction, photon emission and energy exchange coupling between the molecule and spherical leads. As a central result, we report on a three order of magnitude enhanced molecular photon emission, which dependence on molecular and junction parameters are also discussed.

[1] Y. Zelinskyi, Y. Zhang, and V. May, J. Phys. Chem. A, DOI: 10.1021/jp305505c
[2] Y. Zhang, Y. Zelinskyy, and V. May, J. Phys. Chem. C, accepted
[3] Y. Zhang, Y. Zelinskyy, and V. May, J. Nanophot., in press
[4] Y. Zelinskyy and V. May, Nano Lett. **12**, 446 (2012)

CPP 21.5 Wed 10:30 H2

Dynamics of a nano-scale rotor driven by single-electron tunneling — Alexander Croy[2] and •Alexander Eisfeld[1] — [1]MPIPKS Dresden — [2]Chalmers University of Technology S-412 96 Göteborg, Sweden

We investigate theoretically the dynamics and the charge transport properties of a rod-shaped nano-scale rotor, which is driven by a similar mechanism as the *nanomechanical single-electron transistor (NEMSET)*. We show that a static electric potential gradient can lead to self-excitation of oscillatory or continuous rotational motion. We identify the relevant parameters of the device and study the dependence of the dynamics on these parameters. We discuss how the dynamics are related to the measured current through the device. Notably, in the oscillatory regime we find a negative differential conductance. The current-voltage characteristics can be used to infer details of the surrounding environment which is responsible for damping.

[1] A. Croy and A. Eisfeld, *EPL (Europhys Lett)* **98**, 68004

CPP 21.6 Wed 10:45 H2

First-principles investigation of electron transport through molecular junctions in an STM configuration — •Shigeru Tsukamoto, Vasile Caciuc, Nicolae Atodiresei, and Stefan Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich

Molecular electronics is exciting by the perspective that various types of functionalities are potentially realized only by single molecules with unique electronic structures. A number of interesting experiments on the transport properties have been performed in an STM configuration, in which a probing tip approaches a molecule on a metal surface.

By means of first-principles methods, we report about a systematic series of calculations on electron transport through molecules in the STM configuration. The molecules to be investigated are a Terephthalic acid molecule and its derivatives, which chemisorb on Cu(110) surfaces.

Electron transmissions are investigated by varying the tip–molecule distance in an STM configuration, as well as by tuning molecular electronic structures. As approaching the tip toward the molecule, some of the transmission peaks originating from unoccupied states move to lower energy due to the hybridization of tip and molecular states. This peak-shift contributes to increasing the electron transmission around the Fermi energy, which is an essential property in molecular devices. This exhibits that in molecular electronics, not only the molecule itself but also the geometrical configuration between a molecule and the electrodes is an important parameter to determine the functionality.

15 min. break

CPP 21.7 Wed 11:15 H2

STM theory for π-conjugated molecules on thin insulating films — •Benjamin Siegert, Andrea Donarini, Sandra Sobczyk, and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg

We present a microscopic STM theory, based on the reduced density matrix formalism, which is able to describe transport and topographical properties of interacting π-conjugated molecules on thin insulating films. Simulated current-voltage characteristics and constant height

and constant current STM images for a Cu-Phthalocyanine (CuPc) molecule are presented as experimentally relevant examples. We predict negative differential conductance resulting from interference between degenerate many-body states of CuPc [1]. Criteria are given to find and identify the interference blocking scenario in experimental measurements.

[1] A. Donarini, B. Siegert, S. Sobczyk, and M. Grifoni, PRB **86**, 155451 (2012).

CPP 21.8 Wed 11:30 H2

Influence of Electronic Properties of Graphene on Current-Voltage Characteristics of Molecule-Graphene Nanojunctions — •Ivan A. Pshenichnyuk, Pedro B. Coto, André Erpenbeck, and Michael Thoss — Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany

Graphene, thanks to its peculiar mechanical and electronic properties, is today considered as a perspective material in future electronics. Its well-known band structure with "zero band-gap" as well as the existence of so-called edge states leads to a non-trivial density of states distribution in graphene-based devices. This causes, in particular, distinctive current-voltage characteristics of molecule-graphene nanojunctions, where a single molecule is connected to two graphene nanosized contacts. We study the transport characteristics of graphene-based nanojunctions using tight-binding models and first-principles DFT calculations combined with the Landauer transport formalism.

CPP 21.9 Wed 11:45 H2

Electron Transport properties of metallic carbon nanotubes with metal contacts — •Andreas Zienert[1], Jörg Schuster[2], and Thomas Gessner[1,2] — [1]Center for Microtechnologies, Chemnitz University of Technology, Chemnitz, Germany — [2]Fraunhofer Institute for Electronic Nano Systems, Chemnitz, Germany

Metallic carbon nanotubes (CNTs) are quasi ballistic one-dimensional conductors capable to carry large current densities. This makes them ideal candidates for applications in future microelectronic devices, partially replacing state-of-the-art copper interconnect lines. The performance of such a system not only depends on intrinsic properties of the CNTs but is also strongly affected by its size and the contact.

We investigate the transport properties of metal–CNT–metal devices theoretically, applying semiempirical (extended Hückel theory) and ab initio (density functional theory) electronic structure methods, combined with a Green's function formalism for ballistic transport at low bias. The study focuses on $(6, 0)$ CNTs of different length comparing the metal contacts Al, Cu, Pd, Pt, Ag, Au in a highly symmetric end-to-end configuration.

It turns out that Al forms the most transparent contacts, followed by Pd, Pt and Cu. The noble metals Au and Ag perform worse. Results are visualized and discussed in terms of the local density of states of the combined metal–nanotube systems and its isolated parts, as well as their contact distances, binding energies, and work functions.

CPP 21.10 Wed 12:00 H2

First principles study of charge and heat transport through π-stacked molecules — •Thomas Hellmuth[1], Marius Bürkle[2], Fabian Pauly[3], and Gerd Schön[1] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Nanosystem Research Istitute, National Institute of Advanced Industrial Science and Technology, Japan — [3]Theorie der Nanostrukturen, Universität Konstanz, 78457 Konstanz, Germany

We analyze charge and heat transport properties of π-stacked, multilayered paracyclophane molecules using density functional theory combined with non-equilibrium Green's function techniques. The conductance of that class of molecules was measured in Ref. 1. Beside the elastic conductance we investigate the not yet measured thermopower and inelastic electron tunneling spectra (IETS). The transmission eigenchannels show that the current is mainly carried by the π system of the paracyclophane molecules and by taking into account different contact geometries, we find that this is independent of the binding motif. While the conductance decays exponentially with increasing molecular length, the thermopower increases linearly and may change its sign. Similarly, we analyze how the IETS and the heat transport depend on the molecular length and vibrational modes in the specific junction geometries.

[1] S. T. Schneebeli *et al.* J. Am. Chem. Soc. **133**, 2136 (2011)

CPP 21.11 Wed 12:15 H2

Spin selective transport in chiral systems — •Rafael Gutierrez, Thomas Brumme, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany

Recent experiments have demonstrated that the transmission of electrons through layers of chiral molecules can be strongly spin-dependent [1,2]. Here, we extend a previous model [3] to discuss the interrelation between the observed effect and the presence of a spin-orbit coupling interaction induced by helical electrostatic fields. Hereby, we present a minimal model Hamiltonian based on a representation of the Schroedinger equation on a helical pathway and discuss the influence of several parameters on the spin polarization. Complementary to it, full 3D wave packet propagation is discussed in the presence of spin-orbit coupling. Our results suggest that a spin polarization can be induced as a result of the symmetry of the system. However, it appears that a full 3D description of the problem may be necessary.

[1] B. Goehler, V. Hamelbeck, T. Z. Markus, M. Kettner, G. F. Hanne, Z. Vager, R. Naaman, H. Zacharias, Science **331**, 894 (2011)
[2] Z. Xie, T. Z. Markus, S. R. Cohen, Z. Vager, R. Gutierrez, R. Naaman, Nano Letters **11**, 4652 (2011)
[3] R. Gutierrez, E. Diaz, R. Naaman, G. Cuniberti, Phys. Rev. B **85**, 081404(R) (2012)

CPP 21.12 Wed 12:30 H2

Full ab initio description of strong electronic correlations in molecular devices — •David Jacob — Max-Planck-Institut für Mikrostrukturphysik, Halle

In order to obtain a *full* first-principles description of the correlated electronic structure and transport properties of nanoscopic devices we combine the so-called Coulomb-Hole-Screened-Exchange (COHSEX) approximation with more sophisticated many-body techniques such as the Dynamical Mean-Field Theory (DMFT). While the former yields an effective mean-field description of the weakly correlated conduction electrons, the latter describes the dynamic correlations of the strongly interacting electrons in the $3d$- or $4f$-shells of transition metal atoms. The combination of DMFT with COHSEX instead of Density Functional Theory (DFT) improves upon our recently developed "Molecular DMFT" approach [1,2] in two important aspects: First, the COHSEX yields the effective Coulomb interaction U for the strongly interacting electrons. Second, unlike in DFT+DMFT calculations the double-counting correction for COHSEX+DMFT is exactly known and straight-forward to calculate. With this approach it is now possible to actually predict e.g. the occurance of the Kondo effect in magnetic atoms and molecules on metal surfaces and attached to metallic leads, and to investigate the complex nature of the Kondo effect in these sytems.

[1] D. Jacob *et al.*, PRL **103**, 016803 (2009); PRB **82**, 195115 (2010)
[2] M. Karolak *et al.*, PRL **107**, 146604 (2011)