TT 6: Nanoelectronics III - Molecular Electronics

Time: Monday 14:00–17:00 Location: H19

TT 6.1 Mon 14:00 H19

Electron transport through organic molecules and the influence of adsorbates on the conductance of aluminium contacts — •F. Pauly[1,2], S. Wohlthat[1,2], J. Viljas[1,2], M. Häfner[1,2], J.C. Cuevas[1,2,3], and Gerd Schön[1,2] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe — [2]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, D-76021 Karlsruhe — [3]Departamento de Física Teórica de la Materia Condensada C-V, Universidad Autónoma de Madrid, E-28049 Madrid

In the first part of this talk we will analyze the electrical conductance properties of a series of organic molecules. This series comprises molecules with different numbers of phenyl rings and modified side groups [1]. For these oligophenylenes we investigate the changes in the conductance due to both varied molecule lengths and different bonding positions within our newly developed DFT transport program [2,3]. As a second application of our method we study the transport properties of atomic-sized aluminium contacts in the presence of oxygen molecules, namely O, O_2, and O_3. In particlar we analyze the evolution of the transport characteristics for increasing electrode distances, simulating the opening of a break junction [4].

[1] M. Elbing, PhD Thesis, FZ Karlsruhe (2005); [2] F. Pauly, PhD Thesis, Universität Karlsruhe (2007); [3] F. Pauly, J.K. Viljas, U. Huniar, M. Häfner, J.C. Cuevas, and Gerd Schön, (in preparation); [4] S. Wohlthat, Diploma thesis, Universität Karlsruhe (2006)

TT 6.2 Mon 14:15 H19

Nonequilibrium resonant spectroscopy of molecular vibrons — •Dmitry Ryndyk and Gianaurelio Cuniberti — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg

Quantum transport through single molecules is essentially affected by molecular vibrations. We investigate the behavior of the molecular transistor with intermediate electron-vibron coupling and arbitrary coupling to the leads. We have developed a theory which allows to explore this regime via the nonequilibrium Green function formalism parallel to the widely used master equation technique. The problem is motivated by recent scanning tunneling spectroscopy experiments. We show that the nonequilibrium resonant spectroscopy is able to determine the energies of molecular orbitals and the spectrum of molecular vibrations. Our results are relevant to STS experiments, and demonstrate the importance of the systematic and self-consistent investigation of the effects of the vibronic dynamics onto the transport through single molecules.

TT 6.3 Mon 14:30 H19

Influence of vibrational modes on the electronic properties of DNA — •Benjamin Schmidt[1,2], Matthias Hellter[2], Gerd Schön[1,2], Evgeni Starikov[2], and Wolfgang Wenzel[2] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Postfach 3640, 76021 Karlsruhe, Germany

We investigate the electron (hole) transport through short double-stranded DNA wires in which the electrons are strongly coupled to the specific vibrational modes (vibrons) of the DNA. We analyze the problem starting from a tight-binding model of DNA, with parameters derived from ab-initio calculations, and describe the dissipative transport by equation-of-motion techniques. For homogeneous DNA sequences like Poly- (Guanine-Cytosine) we find the transport to be quasi-ballistic with an effective density of states which is modified by the electron-vibron coupling. At low temperatures the linear conductance is strongly enhanced, but above the 'semiconducting' gap it is affected much less. In contrast, for inhomogeneous ('natural') sequences almost all states are strongly localized, and transport is dominated by dissipative processes. In this case, a non-local electron-vibron coupling influences the conductance in a qualitative and sequence-dependent way.

TT 6.4 Mon 14:45 H19

Influence of chopped laser light onto the electronic transport through atomic-sized contacts — •Daniel Guhr, Dennis Rettinger, Johannes Boneberg, Artur Erbe, Paul Leiderer, and Elke Scheer — University of Konstanz, Germany

In our experiment we investigate the influence of laser irradiation onto the electrical conductance of gold nanocontacts established with the mechanically controllable breakjunction technique. We concentrate on the study of reversible conductance changes which can be as high as 200%. In our measurements we have varied the intensity, the polarisation and the wavelength of the laser beam in the visible range of the spectrum as well as its position on the sample. Under most conditions an enhancement of conductance is observed. We discuss several physical mechanisms which might contribute to the observed effect including thermal expansion, rectification of nonlinear current-voltage characteristics by the ac electric field of the laser light [1] and photon-assisted transport (PAT) [2]. From the analysis of our data we conclude that PAT is the dominating effect in out experiment while small contributions from thermal expansion cannot be excluded [3].

[1] R. Möller,J. Vac. Sci. Technol. B9, 506-509, 1991
[2] J.K. Viljas and J.C. Cuevas, cond-mat/0607505
[3] D. Guhr et al., cond-mat/0612117

TT 6.5 Mon 15:00 H19

Role of electronic structure in photo-assisted transport through atomic-sized contacts — •Janne Viljas[1,2] and Juan Carlos Cuevas[1,2,3] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe — [2]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, D-76021 Karlsruhe — [3]Departamento de Física Teórica de la Materia Condensada C-V, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

We study theoretically quantum transport through laser-irradiated metallic atomic-sized contacts [1]. The radiation is treated classically, assuming its effect to be the generation of an ac voltage over the contact. We derive an expression for the dc current and compute the linear conductance in ideal one-atom thick contact geometries as a function of the ac frequency, concentrating on the role played by electronic structure. In particular, we present results for three metals (Al, Pt, and Au), the electronic structures of which are described with an *spd* tight-binding parametrization. Depending on the frequency and the metal, the ac voltage can either enhance or reduce the conductance. This can be intuitively understood in terms of the energy dependence of the transmission in the absence of radiation. Recent experiments [2] on laser-irradiated gold contacts support the view that photo-assisted processes may play an important role in the transport through such systems.

[1] J. K. Viljas and J. C. Cuevas, cond-mat/0607505.
[2] D. Guhr, D. Rettinger, J. Boneberg, A. Erbe, P. Leiderer, and E. Scheer, cond-mat/0612117 and this conference.

15 min. break

TT 6.6 Mon 15:30 H19

Electron transport in bundles of metallic single-walled carbon nanotubes — •Ines Barbara Klugius[1], Christoph Wolfgang Marquardt[1], Frank Hennrich[1], Hilbert v. Löhneysen[2,3], and Ralph Krupke[1] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe, Germany — [2]Universität Karlsruhe, Physikalisches Institut, 76128 Karlsruhe, Germany — [3]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe, Germany

Electron transport in individual metallic single-walled carbon nanotubes (SWNT) has been described within a Luttinger liquid model (LL) which can explain the power law behaviour found in the temperature dependent conductance, as well as in the voltage dependent differential conductance. In heterogeneous bundles of SWNTs, that are composites of metallic and semiconducting tubes, similar power law behaviour has been observed.

During the fabrication of carbon nanotubes both metallic and semicon-ducting ones are produced. Using dielectrophoresis as a method to separate these types, we are able to prepare samples of bundles of exclusively metallic SWNTs. In this configuration, the SWNTs are still surrounded by the surfactant that is necessary for the separation process. On such samples we measure the transport characteristics and anticipate a deviation from the LL behaviour due to enhanced intertube coupling. To enforce the coupling, we anneal the samples assuming that in this manner, the amount of surfactant inbetween the tubes is abated and the tube-tube distance is reduced.

TT 6.7 Mon 15:45 H19

Coulomb repulsion effects in driven electron transport through molecules — •Franz J. Kaiser, Peter Hänggi, and Sigmund Kohler — Institut für Physik, Universität Augsburg, 86135 Augsburg

We investigate the influence of strong Coulomb repulsion on the current through molecular wires. The molecule is described by a tight-binding model whose first and last site is coupled to a respective lead. The leads are eliminated within a perturbation theory yielding a master equation for the wire. In the non-driven case, we explore the transport properties of a bridged molecular wire, where the current decays exponentially as a function of the wire length [1]. For studying conductors driven by external electromagnetic fields, we decompose the reduced density operator into a Floquet basis. This enables an efficient treatment of the time-dependent transport problem. For the electronic excitations in bridged molecular wires, we find that strong Coulomb repulsion significantly sharpens resonance peaks which broaden again with increasing temperature [2].

[1] F.J. Kaiser, M. Strass, S. Kohler, and P.Hänggi, Chem. Phys. **322**, 193 (2006)

[2] F.J. Kaiser, P.Hänggi, and S. Kohler, Eur. Phys. J. (in press); cond-mat/0606457

TT 6.8 Mon 16:00 H19

Multishell Coulomb blockade in multiwall carbon nanotubes — •Emiliano Pallecchi[1], Shidong Wang[1], Csilla Miko[2], Laszlo Forro[2], Milena Grifoni[1], and Christoph Strunk[1] — [1]University of Regensburg, D-93040 Regensburg, Germany — [2]FBS Swiss Federal Institute of Technology (EPFL), CH-1015 Lausanne, Switzerland

We performed low temperature measurements of magnetoconductance and non linear conductance for multiwall carbon nanotubes. Signatures of phase coherent diffusive transport are the weak localization dip and universal conductance fluctuations. At very low temperature, "anomalous" Coulomb blockade is observed: we find a superposition of several diamonds patterns in the Vsd-Ugate plane with different size. The stability diagrams are more regular than in previous studies, but qualitatively different from that observed in single wall carbon nanotubes. We attribute this behavior to the effect of the inner shells on the charging process and propose a model where the nanotube is represented by two quantum dots in parallel.

TT 6.9 Mon 16:15 H19

One dimensional organometallic wires: electronic structure and transport properties — •Volodymyr Maslyuk[1], Alexei Bagrets[2], Mads Brandbyge[3], and Ingrid Mertig[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Physical Department, Halle, Germany — [2]Institute of Nanotechnology, Forschungszentrum Karlsruhe, Germany — [3]NanoDTU, MIC-Department of Micro and Nanotechnology, Technical University of Denmark, Lyngby, Denmark

During the last years, organometallic systems have attracted increasing attention. The small size of the molecules and the spin degree of freedom allow us to consider them as independent logic units and think about new electronic devices with unforeseen properties. Here, we focus on multi-decker metal-cyclopentadienyl Met(C5H5) and metal-benzene Met(C6H6) molecules. Recently, we have predicted that a one-dimensional vanadium-benzene wire is a half-metallic ferromagnet and finite V(C6H6) clusters coupled to magnetic leads are working as spin-filter [1]. Moreover, our bias dependence calculations show conservation of the half-metallic properties in a wide voltage window. Using density functional theory and the non-equilibrium Green's-function method, implemented in the TranSIESTA code [2], we have investigated the electronic and transport properties of 1D organometallic wires coupled with Co(100) electrodes. We have also investigated the electron transport through the molecules in the case of antiparallel magnetic configuration of the electrodes and predict an impressive magnetoresistance effect. [1] V. Maslyuk et al., Phys. Rev. Lett 97, 097201 (2006). [2] M. Brandbyge et al. Phys. Rev. B 65, 165401 (2002).

TT 6.10 Mon 16:30 H19

Cotunneling and non-equilibrium magnetization in magnetic molecular monolayers — •Florian Elste[1] and Carsten Timm[2] — [1]Institut für Theoretische Physik, Freie Universität Berlin, Germany — [2]Department of Physics and Astronomy, University of Kansas, USA

We study the interplay of electronic transport through monolayers of magnetic molecules and their non-equilibrium magnetic moment. A master-equation approach going beyond the sequential-tunneling approximation is applied to study the Coulomb-blockade regime. While the current is very small in this case, the magnetization can be switched by an amount of the order of the saturation magnetization by a small change of bias voltage, and without causing the flow of a large current. Inelastic cotunneling processes manifest themselves as steps in the differential conductance, which are accompanied by much larger changes in the magnetization. In addition, the magnetization in the Coulomb-blockade regime exhibits strong signatures of sequential-tunneling processes de-exciting molecular states populated by inelastic cotunneling. We also consider the case of a magnetic single-molecule transistor, finding that cotunneling processes lead to the occurrence of magnetic sidebands below the Coulomb-blockade threshold. In the context of spintronics applications, we investigate effects of additional spin relaxation. Our results show that sufficiently fast spin relaxation washes out the fine structure in the differential conductance and in the magnetization. At the same time, fast spin relaxation, while in general undesirable, can lead to a highly-polarized current in the presence of a magnetic field.

TT 6.11 Mon 16:45 H19

Der Einfluß von Berry-Phasen auf die Leitfähigkeit eines einzelnen Jahn-Teller Moleküls — •Maximilian G Schultz, Tamara S Nunner und Felix von Oppen — Institut f. Theoretische Physik, FU Berlin, Arnimallee 14, 14195 Berlin

Wir studieren die elektronischen Transporteigenschaften eines oktaedrischen Moleküls im Grenzfall schwacher Kopplung an zwei metallische Elektroden. Die Berry-Phase des $E \otimes e$ Jahn-Teller Effekts impliziert eine nichttriviale Auswahlregel in der Tunnelmatrix; die Jahn-Teller Verzerrung selbst induziert starke Verschiebungen im Spektrum der molekularen Schwingungen. In der Mastergleichung, mit der elektronischer Transport durch das System beschrieben wird, entstehen dadurch absorbierende Zustände, die den stationären Strom durch die Elektroden unterdrücken. Dies führt zu einer negativen differentiellen Leitfähigkeit und einer starken Asymmetrie im dI/dV Diagramm bezüglich der Gate-Spannung.