TT 33 Transport - Nanoelectronics III: Molecular Electronics

Zeit: Dienstag 14:00–18:00 Raum: TU H3027

TT 33.1 Di 14:00 TU H3027

A single-molecule diode — Rolf Ochs[1], Mark Elbing[1], Marcel Mayor[1], Max Köntopp[1], Ferdinand Evers[1], and •Heiko B. Weber[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Postfach 3640, D-76021 Karlsruhe — [2]Institut für Angewandte Physik, Universität Erlangen, Staudtstr. 7, 91058 Erlangen

We have designed and synthesized an organic molecule such that it can be used as a diode on the single-molecule level. Individual molecules were contacted employing the mechanically controlled break junction technique. The results show indeed diode-like current-voltage characteristics. In contrast to that, control experiments with similar symmetric molecules did not show significant asymmetries in the transport properties. In order to investigate the underlying transport mechanism, phenomenological arguments are combined with calculations based on density functional theory. It turns out that the physics responsible for the asymmetry has several analogies to that in a p-n semiconductor diode.

TT 33.2 Di 14:15 TU H3027

Electrical transport through DNA molecules under stretching — •Ning Kang, Roman Lehner, Artur Erbe, and Elke Scheer — Department of Physics, University of Konstanz, Germany

Understanding the mechanism of electron motion along DNA is an essential step for the development of DNA-based molecular electronics. However, a number of contradicting findings were reported regarding the electronic properties of DNA. Theoretical calculations have demonstrated that the charge transport through the DNA will be strongly influenced by conformational transitions. To probe this effect, we have measured the resistance of DNA molecules under stretching with the help of the mechanically controllable break junction technique (MCB). Using the break junctions, we are able to fabricate electrodes with nanometer separation and fine-tune the tunneling gap between electrodes down to a resolution in the picometer range. In our experiments, we used 10-nm-long (30 base pairs) DNA with thiol groups at both ends, and stretched continuously the trapped molecules by means of MCB. A discrete two-level resistance switching behavior is observed when changing the distance of the electrodes, which might be related to a conformation transition of the DNA under stretching. To clarify whether the measured signal is from molecules, we also perform the measurements with a specific enzyme that cuts the DNA.

TT 33.3 Di 14:30 TU H3027

Dissipative Effects in the Electronic Transport through DNA molecular wires — •Rafael Gutierrez, Sudeep Mandal, and Gianaurelio Cuniberti — Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg

DNA-based molecular wires have a huge potential for application in molecular electronics. Their electronic transport properties are however not well elucidated. This is mainly due to the extreme sensitivity of charge propagation in DNA to static and dynamic disorder as well as to environmental effects (counterions, water shell, etc). We investigate the influence of a dissipative environment which effectively comprises the effects of counterions and hydration shells, on the transport properties of short DNA wires. For this purpose we use a tight-binding model embedded in a bosonic bath consisting of a collection of harmonic oscillators. In the absence of interactions with the bath, a temperature independent gap opens in the electronic spectrum. Upon allowing for electron-bath coupling the gap becomes temperature dependent. We show that a crossover from semiconducting to metallic behavior in the low-voltage region of the I-V characteristics can be achieved in some parameter regions. The reason is the appearance of bath-induced polaronic states within the electronic bandgap. We further show that the temperature dependence of the transmission near the Fermi energy displays an Arrhenius-like behavior in agreement with recent transport experiments.

TT 33.4 Di 14:45 TU H3027

Characterization of nanoscale molecular junctions — •Artur Erbe[1], Anat de Picciotto[2], Jennifer E. Klare[2], Colin Nuckolls[2], Kirk Baldwin[3], and Robert Willett[3] — [1]Universität Konstanz, FB Phyisk — [2]Columbia University, NY, USA — [3]Lucent Technologies, Bell Labs, NJ, USA

Exploring the electronic possibilities of nanoscale organic materials has become an important challenge as modern lithographical techniques approach ultimate limits. In this regime, the properties of single or a few molecules will dominate the behavior of whole devices. Recent experiments on nanoscale molecular junctions show a large variety of results. Differences in the properties of the molecules themselves cannot fully account for these variations. This fact indicates that contact properties play an important role in the behavior of the whole junction. We present electrical measurements of various types of molecules using an electrical break junction technique. The formation of the junctions relies on electromigration in a narrow gold wire. This technique allows us to test the junctions under varying external conditions. Distinct features are found in the I-V-characteristics at low temperatures indicating that single or a few molecules are contacted. Some of those features can be affected by changes in applied gate voltage. The energy scales associated with these features cannot be explained with molecular properties alone. In order to explain our results we take interactions between the molecules and the contacting metals into account.

TT 33.5 Di 15:00 TU H3027

Electron-phonon interactions in atomic-scale conductors — •Janne Viljas, Fabian Pauly, and Juan Carlos Cuevas — Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe

With the recent advances in nanofabrication techniques it has become possible to manipulate and explore the electronic transport through atomic-scale wires and individual molecules. This has posed an exciting theoretical challenge, namely the understanding of the conduction mechanisms at the molecular scale. So far, the effort has been mostly concentrated on analysing the role of the electronic structure of the atomic-scale conductors, but little has been done on the role of their internal degrees of freedom. In this talk I will present our efforts to understand what are the effects of the vibrational modes on conduction at the atomic scale. In particular, making use of a tight-binding approach, we describe the influence of the inelastic electron-phonon processes in metallic atomic wires. This allows us to address many different questions such as (i) what determines that in some experimental situations the vibrational modes enhance the current and in some others they reduce it? (ii) What are the possible signatures of these modes in the current-voltage characteristics? (iii) What are the selection rules that explain why some vibrational modes do not show up in the transport experiments?

TT 33.6 Di 15:15 TU H3027

Electron-phonon coupling mechanisms in molecular electron transport — •Michael Hartung and Gianaurelio Cuniberti — Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

We study the conductance through a single vibrating molecule contacted to two metallic electrodes. The starting point is a tight-binding Hamiltonian with a linear coupling of the ionic motion to the electronic degrees of freedom. We distinguish between a coupling to the *onsite* energy of the molecule and a coupling representing a *bond-stretching* vibrational mode.

The full nonequilibrium current, shot noise, and dissipated power is calculated within the Keldysh Green function formalism. As far as transport observables are concerned, onsite and bond-stretching coupling mechanisms differ in several respects: In the latter case satellite peaks in the differential conductance are more pronounced and results closer to the experimental evidence can be obtained.

TT 33.7 Di 15:30 TU H3027

Vibrational effects in transport through a few level molecule. — •Dmitri Ryndyk — Universität Regensburg

We consider a simple molecule with several electron levels placed between large metallic leads. At finite voltage internal vibrations of the molecule as well as an oscillation of the whole molecule between the leads can be excited. We use the self-consistent nonequilibrium theory to describe electron transport through a molecule and dynamics of vibrations. At small voltage or high temperature current is affected by thermally excited vibrations. At larger voltage and low enough temperature transition into the regime with nonequilibrium vibrations is possible. Phase diagram of the system is controlled by coupling to the leads, electronvibron coupling, and coupling of vibrations to the thermal bath. The other nonequilibrium effect which should be taken into account is spectrum modification due to nonequilibrium distribution function of electrons at finite voltage.

Pause

TT 33.8 Di 16:00 TU H3027

Theoretical analysis of conductance histograms of Au atomic contacts — •F. Pauly[1], M. Dreher[2], J.C. Cuevas[1], E. Scheer[2], and P. Nielaba[2] — [1]Institut für Theoretische Festkörperphysik, University of Karlsruhe, 76128 Karlsruhe, Germany — [2]Physics Department, University of Konstanz, 78457 Konstanz, Germany

Many experiments have shown that the conductance histograms of metallic atomic-sized contacts exhibit a peak structure, which is characteristic of the corresponding material. In order to shed some light on the origin of these peaks, we present a theoretical analysis of the conductance histograms of Au atomic contacts, investigating the interplay between mechanical and electrical properties of these nanocontacts. We have combined classical molecular dynamics simulations of the breaking of nanocontacts with conductance calculations based on a tight-binding model. This combination gives us access to crucial information such as contact geometries, forces, minimum cross section, total conductance and transmission coefficients of the individual conduction channels. We also compare with experimental results on Au atomic contacts where the individual channel transmissions have been determined.

TT 33.9 Di 16:15 TU H3027

Utilization of Carbon Nanotubes by Surface Acoustic Waves — •Jens Ebbecke[1], Christoph J. Strobl[2], and Achim Wixforth[1] — [1]Institut für Physik der Universität Augsburg, Experimentalphysik I, Universitätsstr. 1, 86135 Augsburg — [2]Sektion Physik der Ludwig-Maximilian-Universität und Center for Nanoscience (CeNS), Geschwister-Scholl-Platz 1, 80539 München

We report a surface acoustic wave (SAW) mediated carbon nanotube (CNT) alignment parallel to the sample surface. The piezoelectric field of the SAW aligns the CNTs in parallel to the wave vector. Furthermore we have contacted single-walled CNTs after aligning them. The acoustoelectric current has been measured at 4.2 K and a probing of the low-dimensional electronic states by the SAW has been detected. By decreasing the acoustic wavelength resulting in an adjustment to the length of the defined CNT constriction a quantization of the acoustoelectric current has been observed.

TT 33.10 Di 16:30 TU H3027

Magnetoconductance in Disordered Carbon-Nanotubes — •Norbert Nemec and G. Cuniberti — Molecular Computing Group, Universität Regensburg, Germany

Single wall carbon-nanotubes in tight-binding approximation are one of the simplest nontrivial theoretical models with physical relevance that can be used for studying quantum mechanical transport mechanisms at the molecular scale. Based on this this model, we examine the interplay of disorder with external magnetic fields, leading to signs of weak localization. As expected, weak localization is enhanced in the energy regions with high density of states. We quantify the resulting energy dependent mean free path in relation to the sample size and the strength of the disorder. “Coating wideband leads” are introduced as a novel approach to model realistic contacts as they are found in experiment, without adding much computational complexity.

TT 33.11 Di 16:45 TU H3027

Non-linear transport properties in commensurate and incommensurate double-walled carbon nanotubes — •Shidong Wang and Milena Grifoni — Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

We use a tight-binding model to investigate the effective intershell coupling in double-walled carbon nanotubes. We derive an analytical expression for the effective intershell coupling and find selection rules. The intershell coupling between lowest bands is significantly suppressed if two shells are incommensurate. Including the long-ranged Coulomb interactions, double-walled carbon nanotubes can be described by Luttinger liquid theory at low energies. The tunneling density of states and the non-linear I-V characteristics of double-walled carbon nanotubes are also obtained.

TT 33.12 Di 17:00 TU H3027

Franck-Condon blockade and giant Fano factors in transport through single molecules — •Jens Koch and Felix von Oppen — Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

We show that Franck-Condon physics leads to a significant current suppression at low bias voltages (termed Franck-Condon blockade) in transport through single molecules with strong coupling between electronic and vibrational degrees of freedom.

For weak vibrational relaxation, we find that transport in this regime is characterized by remarkably large Fano factors (10^2–10^3), which arise due to avalanche-like transport of electrons. Avalanches occur in a self-similar manner over a wide range of time scales, as reflected in power-law dependences of the current noise on frequency and vibrational relaxation rate.

TT 33.13 Di 17:15 TU H3027

Transport calculations for single molecules based on density functional theory: some fundamentals — •F. Evers[1], K. Burke[2], and R. Gaudoin[2] — [1]Institut für Nanotechnologie, Forschungszentrum Karlsuhe, 76021 Karlsruhe, Germany — [2]Department of Chemistry and Chemical Biology, Rutgers University, 610 Taylor Road, Piscataway NJ 08854

In principle, the use of time dependent density functional theory (TDDFT) allows for exact calculations of the linear and non-linear density and current response of interacting many-body systems. An important application of this method are transport calculations for single molecules. In practice, one is forced to make approximations for the exchange correlation (XC) functional employed which then can put serious limits to the accuracy of TDDFT calculations. We will discuss artifacts that can occur if the non-equilibrium XC-functional is replaced by the equilibrium one. A formalism will be proposed that allows to include the XC-functional in the hydrodynamic approximation (Vignale and Kohn) into the standard DFT-approach to transport.

TT 33.14 Di 17:30 TU H3027

Electron and Exciton Transfer in Donor-Acceptor Systems: Many-Particle Effects and Influence of Electronic Correlations — •Sabine Tornow, Ning-Hua Tong, and Ralf Bulla — Theoretische Physik III, Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

The spin boson model provides a well established description of electron transfer processes from a donor to an acceptor. The redox sites are modelled by two localized quantum states. This picture breaks down in multi electron transfer processes if many particle effects and electron correlations have to be taken into account. We present a theoretical nonperturbative study of the electron and exciton transfer based on an extended spin boson model where the redox sites are modelled more realistically. Using Wilsons Numerical Renormalization Group method we discuss effects of the electron correlations on the transfer rate.

TT 33.15 Di 17:45 TU H3027

Magnetic Field Dependent Band Structure in Multiwall Carbon Nanotubes — •Bernhard Stojetz[1], Francois Triozon[2], Stephan Roche[2], Lazlo Forró[3], and Christoph Strunk[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg — [2]Commissariat à l’Énergie Atomique, DRFMC/SPSMS, 38042 Grenoble, France — [3]Institute of Physics of Complex Matter, FBS Swiss Federal Institute of Technology (EPFL), Lausanne, Switzerland

We report conductance measurements for large diameter (30 - 40 nm) individual multiwall carbon nanotubes in magnetic fields both parallel and perpendicular to the tube axis. A prestructured Al backgate allows a substantial shift of the Fermi level. The thin native oxide on the Al films provides a very efficient electrostatic coupling between the gate and the tube.

The conductance of the nanotube was recorded as a function of the magnetic field B and the gate voltage U. For parallel fields, both h/e- and $h/2e$-periodic oscillations in the magnetoconductance occur and lead to rhomb-shaped regions of low conductance in the B-U-plane . In the perpendicular case, a region of low conductance forms at small gate voltges, which grows with increasing magnetic field.

The experimental observations are explained well by tight- binding bandstructure calculations for the outermost shell of a multiwall nanotube in a magnetic field.