TT 9 Transport: Nanoelectronics III - Molecular Electronics

Time: Monday 14:00–17:45 Room: HSZ 304

TT 9.1 Mon 14:00 HSZ 304

Franck-Condon blockade beyond sequential tunneling — •Jens Koch[1], Felix von Oppen[1], and A. V. Andreev[2] — [1]Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Department of Physics, University of Washington, Box 351560, Seattle, WA 98195, U.S.A.

Recent studies of electronic transport through single-molecule devices have revealed that the coupling of electronic degrees of freedom to a well-defined mode of molecular vibrations may result in a significant current suppression (Franck-Condon blockade). This effect also has characteristic consequences for Fano factors and noise spectra. However, similar to the case of Coulomb blockade, higher-order processes beyond sequential tunneling may become relevant in the blockade regime. Here, we discuss the effects of such corrections on the current-voltage characteristics and noise properties of the system.

TT 9.2 Mon 14:15 HSZ 304

Electromechanical properties of a biphenyl transistor — •Andrea Donarini, Utpal Sarkar, Milena Grifoni, and Klaus Richter — Theoretische Physik, Universitätsstraße 31, D-93053 Regensburg

Electrical transport through gated single molecules (also called molecular transistors) has become since a few years an active research field both theoretically and experimentally [1]. We investigate the interplay between electrical and mechanical degrees of freedom in transport across a biphenyl molecule in the Coulomb blockade regime. In particular, we analyze the role played in the electrical transport by the twisting mode between the phenyl rings. At low biases we can restrict our analysis to the neutral and anionic (one extra electron) state of the molecule only. The neutral molecule has two stable configurations at finite dihedral angles ($\theta \approx \pm\pi/4$) while the anion state is planar. Charge transitions between the electrical states are thus modulated by Franck Condon amplitudes that account for the torsional degree of freedom yielding big phonon blockade effects [2]. We study the system using a generalized master equation for the reduced density matrix. We find that, due to the mechanically degenerate neutral state, the coherencies and not only the populations of the reduced density matrix determine the transport characteristics [3].

[1] A. Yacoby *et al.* Nature **436**, 677 (2005)
[2] J. Koch, F. von Oppen, Phys. Rev. Lett. **94**, 206804 (2005)
[3] A. Donarini, U. Sarkar, M. Grifoni and K. Richter in preparation

TT 9.3 Mon 14:30 HSZ 304

Controlled Nanogap Manufacturing for Single Molecule Contacts by Electromigration — •Veit Wagner, Arne Hoppe, and Jörg Seekamp — International University Bremen

Electrical measurements of single molecules require a pair of electrodes separated by a nanogap of only a few nanometers. Many preparation methods lack the possibility to form an additional gate electrode. We report on nanogap formation by electromigration using the substrate as additional gate electrode. A small metal wire of typically 100 nm width is broken by imposing a high current density at l-He temperature. At room temperature (RT) this approach usually leads to gaps much larger than molecular sizes. Recently Strachan et al. reported on successful nanogap production at RT by using an active control scheme for the applied voltage in dependence of the measured conductivity of the wire. Following this approach we present an alternative control scheme, which includes in addition the time derivative of the conductivity and the average noise level. Gold nanowires of 100 nm width and 20nm height with a Ti adhesion layer on a SiO2-surface were prepared by e-beam lithography. A current level of about 5 mA is usually sufficient to start the electromigration process at room temperature. We test different wire shapes, e.g. a long thin wire of constant thickness or a thick wire with a lithographically defined short narrowing. We find the long thin wire to be more demanding for our control loop than a wire with a short narrowing. The regulation behavior of our control loop for various regions of the process is discussed. With our approach we can reproducibly manufacture gaps at RT with gap sizes smaller than 10 nm.

TT 9.4 Mon 14:45 HSZ 304

Atomic-Scale Quantum Switches: An Approach towards Quantum Electronics at Room Temperature — •Thomas Schimmel[1,2], Fangqing Xie[1], and Christian Obermair[1] — [1]Institute of Applied Physics, University of Karlsruhe, D-76128 Karlsruhe, Germany — [2]Institute of Nanotechnology (INT), Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany

Using a novel electrochemical approach, we demonstrate the fabrication of bistable atomic-scale metallic point contacts, which can be reproducibly opened and closed by means of a voltage applied to an independent third electrode used as a gate electrode [1]. In this way, an electrical circuit can be opened and closed by the controlled and reproducible reconfiguration of the contacting atoms. After the fabrication of the atomic-scale contact by electrochemical deposition of silver within a nanoscale gap, the bistable configuration of the contact is achieved by an electrochemical cycling process. When the contact is closed, is shows conductance quantization, the conductance being $G_0 = 2e^2/h$ or predefined multiples of this value, the on-state conductance being controlled by the cycling parameters. The device reproducibly operates at room temperature. It represents a first demonstration of an atomic relay or transistor, opening intriguing perspectives for the emerging fields of quantum electronics and logics on the atomic scale.

[1] F.-Q. Xie, L. Nittler, Ch. Obermair and Th. Schimmel, Phys. Rev. Lett. 93, 128303 (2004).

TT 9.5 Mon 15:00 HSZ 304

Spin-dependent transport through individual carbon nanotubes — •Emiliano Pallecchi[1], Dominik Preusche[1], Elsa Thune[1], Benoit Witkamp[2], Alberto Morpurgo[2], and Christoph Strunk[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]Kavli Institute of Nanoscience, TU Delft, Netherlands

We report on experiments on carbon nanotubes (CNTs) with ferromagnetic contacts made from $Pd_{0.6}Fe_{0.4}$ alloys. The nanotubes and the micromagnetic properties of the contacts have been characterized by high resolution TEM and Lorentz-microscopy. We have performed low temperature magnetoconductance measurements on individually contacted CNTs as a function of gate voltage and magnetic field. From the weak localization effect in multiwall CNTs we get a signature of the band structure. The low field magnetoconductance shows a hysteretic switching behavior that we attribute to the magnetization reversal of the contacts. The amplitude of the low-field magnetoconductance varies strongly with gate voltage.

TT 9.6 Mon 15:15 HSZ 304

Electron transport in bundles of metallic single-walled carbon nanotubes — •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

Concerning the electronic transport properties, an individual metallic single-walled carbon nanotube (SWNT) has been described as a Luttinger liquid system (LL). This regime can describe the power law behaviour found in the temperature dependent conductance, as well as in the voltage dependent differential conductance [1]. In heterogeneous bundles of SWNTs, that are composite bundles of metallic and semiconducting tubes, similar power law behaviour has been observed [2], which implies, that the metallic tubes in a heterogeneous bundle are well decoupled from each other by the semiconducting nanotube matrix. During the fabrication of carbon nanotubes both metallic and semiconducting ones are produced. Using dielectrophoresis as method to separate these types [3], we are able to prepare samples of bundles of exclusively metallic SWNTs, i.e. without the semiconducting nanotube matrix. Here we present measurements of the transport characteristics of such samples, that show obvious deviation from the LL behaviour.

[1] M. Bockrath et al., Nature 397 (1999) 598 [2] R. Krupke et al., Nano Lett. 3 (2003) 1019 [3] R. Krupke et al., Science 301 (2003) 344

TT 9.7 Mon 15:30 HSZ 304

Contact dependence of carrier injection in carbon nanotubes: An *ab initio* study — •Norbert Nemec[1], David Tománek[2], and Gianaurelio Cuniberti[1] — [1]Institut für theoretische Physik, Universität Regensburg, 93040 Regensburg — [2]Physics and Astronomy Department, Michigan State University, East Lansing, Michigan 48824-2320

We combine *ab initio* density functional theory with transport calculations to provide a microscopic basis for distinguishing between 'good' and 'poor' metal contacts to nanotubes. Comparing Ti and Pd as examples of different contact metals, we trace back the observed superiority of Pd to the nature of the metal-nanotube hybridization. Based on large scale Landauer transport calculations, we suggest that the 'optimum' metal-nanotube contact combines a weak hybridization with a large contact length between the metal and the nanotube.

TT 9.8 Mon 15:45 HSZ 304

Scaling law for the conductance of gold nanotubes — •Miriam del Valle[1,2], Carlos Tejedor[1], and Gianaurelio Cuniberti[2] — [1]Dpto. Física de la Materia Condensada, Universidad Autónoma de Madrid, Spain — [2]Institute of Theoretical Physics, Universität Regensburg, Germany

A new form of gold nanobridges has been recently observed in ultrahigh-vacuum experiments, where the gold atoms rearrange to build helical nanotubes, akin in some respects to carbon nanotubes. The good reproducibility of these wires and their unexpected stability will allow for conductance measurements and make them promising candidates for future applications . We present here a study of the transport properties of these nanotubes in order to understand the role of chirality and of the different orbitals in conductance. The conductance per atomic row shows a light decreasing trend as the diameter grows, which can be also seen through an analytical formula based on a one-orbital model.

— 15 min. break —

TT 9.9 Mon 16:15 HSZ 304

Electron-vibration interactions in transport through atomic gold wires — •Janne Viljas[1], Juan-Carlos Cuevas[1,2,3], Fabian Pauly[1], and Michael Häfner[1] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, Germany — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain — [3]Forschungszentrum Karlsruhe, Institut für Nanotechnologie

The effect of electron-vibration coupling on the conduction through molecular-scale conductors has recently gained considerable attention. Atomic wires formed in metallic point contacts are very simple examples of "molecular"conductors, and are ideal test systems for understanding inelastic transport at the molecular scale. Making use of tight-binding models, we describe the influence of electron-vibration processes on the conductance-voltage characteristic of atomic gold wires [1]. The signature of the excitation of vibrations is usually a series of downward steps. We study systematically how the step heights and voltage positions vary under stretching of wires with varying numbers of atoms, and find a good overall agreement with recent experiments [2].

[1] J. K. Viljas *et al.*, cond-mat/0508470.
[2] N. Agraït *et al.*, Phys. Rev. Lett. **88**, 216803 (2002).

TT 9.10 Mon 16:30 HSZ 304

Nonequilibrium excitations of molecular vibrons — •Dmitry Ryndyk, Michael Hartung, and Gianaurelio Cuniberti — Institute for Theoretical Physics, University of Regensburg, Germany

We consider the nonequilibrium quantum vibrations of a molecule clamped between two macroscopic leads in a current-carrying state at finite voltages. Our approach is based on the nonequilibrium Green function technique and the self-consistent Born approximation. Kinetic equations for the average populations of electrons and vibrons are formulated in the weak electron-vibron coupling case and self-consistent solutions are obtained. The effects of vibron emission and vibronic instability are demonstrated using few-orbital models. The importance of the electron-vibron resonance is shown.

[1] D.A. Ryndyk, M. Hartung, and G. Cuniberti, Phys. Rev. B, to appear; cond-mat/0508143

TT 9.11 Mon 16:45 HSZ 304

Conjugation effects in transport through single-molecule junctions - a theoretical study — •Fabian Pauly[1], J. K. Viljas[1], J. C. Cuevas[1,2,3], and Gerd Schön[1,3] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe — [2]Departamento de Física Teórica de la Materia Condensada C-V, Universidad Autónoma de Madrid — [3]Forschungszentrum Karlsruhe, Institut für Nanotechnologie

Electrical conduction through molecules depends critically on the delocalization of the molecular electronic orbitals and their connection to the leads. Thiolated conjugated molecules are therefore considered good candidates for molecular conductors [1]. Inspired by the recent synthesis of molecules [2] we investigate theoretically the electronic transport through a series of organic molecules, in which the conjugated π-system has either been stabilized or broken by the use of side groups. For the analysis, we use our newly developed transport program based on the DFT quantum chemistry software TURBOMOLE [3].

[1] C. Joachim, J.K. Gimzewski, A. Aviram, Nature 408, 541-548 (2000)
[2] M. Elbing, PhD Thesis, FZ Karlsruhe (2005)
[3] K. Eichkorn, O. Treutler, H. Öhm, M. Häser, and R. Ahlrichs, Chem. Phys. Letters 242, 652 (1995)

TT 9.12 Mon 17:00 HSZ 304

Electronic Transport through C_{60} — •Tobias Böhler, Jochen Grebing, and Elke Scheer — Universität Konstanz

The electronic transport through a single or a few C_{60} molecules is studied experimentally with the help of the mechanically controllable break-junction (MCB) technique [1]. The tip electrodes of the MCB are fabricated of aluminum or gold. The molecule is evaporated onto an opened break-junction under UHV conditions and at low temperatures. At room and low temperature the experiment shows evidence that the conductance of a single C_{60} molecule between gold contacts is in the order of 0,1 G_0. This can be seen in opening and closing curves as well as in time-dependent fluctuations of the conductance. First results of C_{60} between Al electrodes are presented.

[1] T. Böhler et al. Nanotechnology 15 (2004) 465

TT 9.13 Mon 17:15 HSZ 304

Kondo effect in molecular magnets — •Christian Romeike, Maarten R. Wegewijs, Walter Hofstetter, and Herbert Schoeller — ITP A, RWTH Aachen

Motivated by recent experiments by Heersche et al. [1] we investigate linear transport through a single molecular magnet (SMM) in the regime of strong coupling to the electrodes. The molecule is modeled by a spin Hamiltonian incorporating the generic properties of a SMM: an easy-axis anisotropy, an easy-plane anisotropy perturbation leading to the quantum tunneling of magnetic moment (QTM) and a large spin ($S > 1/2$). Using a scaling analyses and the numerical renormalization group we find that for half-integer spin S the molecule acts as an anisotropic, effective pseudo-spin 1/2 Kondo-impurity of which electrons can resonantly scatter. Electron- and spin-tunneling processes *cooperate* to produce a quantum tunneling of the magnetization (QTM) (which is forbidden by time-reversal symmetry for isolated SMMs with half-integer S) and a zero-bias anomaly in conductance. The Kondo temperature is found to depend sensitively on the ratio of the easy-plane and easy-axis anisotropies in a non-monotonic way. We discuss criteria for candidate SMMs for transport experiments.

[1] H. Heersche et al., cond-mat/0510732

TT 9.14 Mon 17:30 HSZ 304

Multifractal energy spectra and anomalous diffusion properties of wave packets in incommensurate double-walled carbon nanotubes — •Shidong Wang and Milena Grifoni — Theoretische Physik, Universität Regensburg, 93053 Regensburg

We calculate the energy spectra of incommensurate doubled-walled carbon nanotubes (DWNTs) by approximating the structures with closely related commensurate ones. The energy spectra show multifractal properties. By using the relation between the moments of wave packets and the multifractal dimensions of the energy spectra (F. Piéchon PRL 76, 4372 (1996)), we obtain the diffusive exponent σ_2, where $\langle x^2 \rangle \sim t^{2\sigma_2}$. The exponent σ_2 strongly depends on the coupling between shells varying from $\sigma \to 1/2$ (diffusive limit) for very strong coupling to $\sigma \to 1$ (ballistic limit) for weak coupling. We compare our results with numerical estimates of σ_2 of wave packets in incommensurate DWNTs (S. Roche et al. PRB 64, 121041 (2001); PLA 285, 94 (2001)), and we obtain very

good quantitative agreement.