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