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TT 8.29 Fr 14:00 Poster TU C

Electronic and Optoelectronic Properties of Single-Molecule Junctions — •Joachim Reichert[1], Cao Qi[1], Harald Fuchs[1], Ivan Stich[2], and Dominik Marx[3] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, D - 48149 Münster — [2]Center for Computational Material Science, Slovak University of Technology, Ilkovicova 3, 812 19 Bratislava — [3]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D - 44780 Bochum

Recent developments and advances in atomic-scale imaging and manipulation techniques enables access to a new field of single molecule experiments. Electronic transport measurements through single organic molecules which are immobilized by self assembling techniques between two metallic electrodes (e.g. mechanically controlled breakjunction [1]) as well as tunnelling experiments through molecular films with STM have proven the ability of organic molecules to act as functional parts in nanoscale-devices. Especially scanning near-field optical microscopy (SNOM) with its ability to apply an optical field to a molecular system in a controlled manner enlarges the range of experimental available properties in metal-anchored molecular junctions. With a combination of these techniques we want to study the electronic/optoelectronic properties of single molecules covalently linked between a metallic substrate and a SNOM-tip to improve the understanding of electronic transport through single molecules.

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TT 8.30 Fr 14:00 Poster TU C

Discrete low-bias conductance fluctuations in molecular break-junctions — •Jan U. Würfel, Mark Elbing, Marcel Mayor, and Heiko B. Weber — Institut für Nanotechnologie, FZ Karlsruhe

We investigate the electronic transport properties of gold-molecule-gold junctions using the mechanically-controllable break-junction (MCBJ) technique. We have shown in former studies that under certain conditions single-molecule contacts could be achieved [1]. Here, we study the longterm stability (up to days) of stable and reproducible contacts, which show discrete transitions in the conductance at low bias ($\sim$ 10 mV). Some of the conductance values could be identified as integer multiples of a fixed value. This may suggest an integer number of molecules contributing. The findings are discussed.

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TT 8.31 Fr 14:00 Poster TU C

A perturbative expansion of shot noise in quantum dots and molecules — •Matthias Hettler[1], Jasmin Aghassi[1,2], Axel Thielmann[1], Jürgen König[3], and Gerd Schön[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie,76021 Karlsruhe, Germany — [2]Institut für Theoretische Festkörperphysik , Universität Karlsruhe, 76128 Karlsruhe, Germany — [3]Institut für Theoretische Physik III, Ruhr-Universität Bochum, 44780 Bochum, Germany

We study current and shot noise in perturbation theory in the coupling of a mesoscopic object (e.g. quantum dot or molecule) to metallic electrodes. We explicitly account for the electronic interactions and the resulting many-body states of the molecule/quantum dots, and allow for relaxation of the excited states. We present in some detail the diagrammatic technique that allows for the computation of the noise to second order in the molecule-electrode coupling. In particular, we discuss the influence of co-tunneling processes as well as the effect of intermolecular (interdot) couplings and relaxation on the shot noise. Furthermore, we find the Fano factor to be very sensitive to the tunnel-coupling strength, which may serve as a spectroscopic tool for the various coupling strengths.

TT 8.32 Fr 14:00 Poster TU C

Nanoscale electrodes on cleaved edge semiconductor surfaces for molecular electronics applications — •Sebastian Strobel[1], Sebastian Luber[1], Dieter Schuh[1], Werner Wegscheider[2], and Marc Tornow[1] — [1]Walter Schottky Institut, TU München, 85748 Garching, Germany — [2]Institut für Angewandte und Experimentelle Physik, U Regensburg, 93040 Regensburg, Germany

Current efforts in molecular electronics target at novel concepts for future nano-electronics thereby aiming at a fundamental understanding of charge transfer mechanism in (bio-) molecular "wires" such as DNA. Starting point is the preparation of suitable nanogap - electrodes that serve as electrical contacts to the molecules.

We present a novel strategy based on a semiconductor heterostructure grown by molecular beam epitaxy that consists of a AlGaAs layer into which a thin layer of GaAs (5 - 20 nm) is embedded. After cleaving the structure an atomically flat plane is obtained. Subsequent selective etching of the GaAs layer perpendicular to that plane and evaporation of a few nanometer thick metal film yields the nano-gap electrodes.

We successfully bridged nano-gap electrodes with single, 30 nm diameter colloidal Au nano-particles by AC electric trapping. The resulting drop in resistance of up to seven orders of magnitude verified the electrical functionality of our devices. First measurements on electrodes functionalized with organic self-assembled monolayers will be presented.

TT 8.33 Fr 14:00 Poster TU C

Multiphoton photofieldemission in electromigrated nanogaps — •S. Dantscher[1], D. Wolpert[1], W. Pfeiffer[1], J. U. Würfel[2], and H. B. Weber[2] — [1]Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg — [2]FZ Karlsruhe, Institut für Nanotechnologie, PO-Box 3640, 76021 Karlsruhe

The combination of nanocontacts and laser excitation offers the possibility of studying photoinduced nonequilibrium transport phenomena and therefore also electron dynamics on the nanometer scale. Using the method of electromigration, contacts with electrode distances in the range of several nanometers can be produced. For relatively large gaps no tunnel current is detectable, i.e. with a moderate applied DC bias, that avoids field emission, these junctions carry no significant current.

We have investigated photocurrents in such contacts under illumination with ultrashort femtosecond laserpulses. The use of a microscope objective as focusing element provides focal radii down to $2\mu m$ resulting in maximum intensities during the pulses of $10^{10} W/cm^2$. Under these conditions and with bias voltages in the range of $\pm$ 5V photo induced currents are detected. The intensity dependences exhibit power laws with exponents up to 3, indicating that multiphoton excitation is responsible for the detected current. Moreover the multiphoton order depends on the actual junction parameters, such as the applied bias. This suggests that the photocurrent flows in the nanogap. The observed bias dependence is attributed to photofieldemission, i.e. the multiphoton photocurrent is influenced by the static field distribution in the gap. In addition, also dynamic field effects might affect the signals.

TT 8.34 Fr 14:00 Poster TU C

Molecular conductance at finite voltage: bias driven evolution of Kohn-Sham-orbitals — •Max Koentopp, Ferdinand Evers, Florian Weigend, Mark Elbing, Rolf Ochs, Marcel Mayor, and Heiko Weber — Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany

Ground state density functional theory calculations yield the exact electron density if the exact exchange-correlation functional is employed.

The evolution of the equilibrium density with parametric changes in the Hamiltonian, e.g. realized by a change in the electrostatic potential, can provide crucial information about transport properties, like the Coulomb blockade.

To test our ideas, we perform model calculations using TURBOMOLE for a diode molecule, which exhibits a structure of a double quantum dot and has been investigated experimentally [1]. In particular, we investigate the origin of the characteristic peak structure in the differential conductance. Our results are consistent with the interpretation that the stepwise increase of the conductance occurs when the number of occupied levels of one of the dots, that have an energy above the lowest unoccupied level of the other dot, increases by one.

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TT 8.35 Fr 14:00 Poster TU C

Manipulating a molecule's conformation with gates: a molecular switch — •Andreas Arnold, Max Koentopp, Ferdinand Evers, and Oliver Rubner — Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany

Molecules can undergo a conformational change when being charged. For molecules connected to external leads their excess charge becomes a parameter that can be tuned by means of a gate. Therefore, the mole-