ric and an asymmetric layout as well as combinations of nonmagnetic electrodes with magnetic bridges and vice versa. In all geometries the MRR is of comparable size and the MR traces show a rich behavior. The main conclusion which we draw from our results is that the micromagnetism of the electrodes as well as the precise atomic arrangement of the contact account for the large MR values.

TT 35.20 Wed 14:00 P1A

Formation of low conductive constrictions in nanostructures by electromigration — •Birgit Kiessig[1,2], Wanyin Cui[1,2], Kai Grube[1], Regina Hoffmann[2], and Roland Schäfer[1] — [1]Forschungszentrum Karlsruhe, IFP, Postfach 3640, 76021 Karlsruhe — [2]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe

Exposure of metallic nanostructures to high currents leads to deterioration by melting or electromigration. Ref. 1 describes a method how to use the latter in a controlled way to form constrictions with conductances down to the conductance quantum $G_0 = 2e^2/h$. Below several G_0 conductance prefers to stabilize at material dependent values well known from conductance quantization experiments.
We apply the method described in Ref. 1 to different materials and extend it to nanostructures containing rings. The rings are connected to two leads at opposite sides and the electromigration-controlled constriction formation acts in a balanced way in both ring arms.
[1] R. Hoffmann, D. Weissenberger, J. Hawecker, and D. Stöffler, Appl. Phys. Lett. **93**, 0431118 (2008).

TT 35.21 Wed 14:00 P1A

Electron induced heating and molecular phonon cooling in single C_{60} junctions — Gunnar Schulze, Katharina J. Franke, and •Jose Ignacio Pascual — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

The functionality of single molecules as electronic devices relies on its stability against large current densities. Electronic current generates heat in the molecular junction due to coupling of electrons with molecular vibrations. Using a scanning tunnelling microscope operated at 5 K, we thermally decompose single C_{60} molecules on a metal surface by passing current through them, and investigate the response of the degrading current (and power) to changes in electron energy. The power for decomposition results from the balance between heating and cooling efficiencies [1]. We find that heating varies with electron energy and reflects the molecular resonance structure participating in the transport. Through inelastic electron spectroscopy measurements, we identify those vibrations which are mostly excited when tunneling through the LUMO state, confirming that symmetry selection rules apply here. Cooling, on the other hand, is a non-resonant process, dominated by the decay of molecular vibrations into electron-hole pair excitations. We find that the partial occupation of molecular states enhance the molecular cooling due to an enhancement of density of states at the molecule-metal interface [2].
[1] G. Schulze, et al., Phys. Rev. Lett. 100, 136801 (2008)
[2] G. Schulze, et al., N. J. Phys. 10, 065005 (2008)

TT 35.22 Wed 14:00 P1A

Quantum Transport Through Gold Wires: Ab Initio Studies Using Plane Waves and Supercells — •Björn Oetzel[1,2], Martin Preuss[1,2], Frank Ortmann[1,2], Karsten Hannewald[1,2], and Friedhelm Bechstedt[1,2] — [1]Institut für Festkörperphysik und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]European Theoretical Spectroscopy Facility, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

We present a numerical scheme for an *ab initio* implementation of the Landauer-Büttiker theory for quantum transport by means of supercells and plane-wave basis sets. The suggested method works entirely in **k** space which allows to circumvent the complicated projections onto tight-binding Hamiltonians necessary in the more common real-space approaches to quantum transport. Here we apply this method to DFT calculations of transmission functions for quasi-1D Au nanowires of various lengths and widths. The results are discussed with respect to the possible replacement of semi-infinite electrodes by short Au nanowires in future calculations of metal-molecule-metal junctions.

TT 35.23 Wed 14:00 P1A

Molecular Switches in Break Junction Metal-Molecule-Metal Contacts — •Bernd Briechle[1], Thomas Kirchner[1], Uta Eberlein[1], Simon Verleger[1], Marcel Mayor[2], Alfred Blaszczyk[2], Thomas Huhn[3], Jannic Wolf[3], Dima Sysoiev[3], Elke Scheer[1], and Artur Erbe[1] — [1]FB Physik, Universität Konstanz, Germany — [2]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe — [3]FB Chemie, Universität Konstanz, Germany

Metal-molecule-metal contacts are established using the Mechanically Controllable Break Junction (MCBJ) technique at room temperature in a toluene solution. We investigate short oligo phenylene ethynylenes (OPE) with various nitrogen-based end groups as well as different thiol-terminated molecular switches. Analysis is based on statistics of conductance traces recorded during opening and closing the junction, and on current-voltage characteristics taken at a constant electrode distance. We show that the latter can be described by a simple transport model involving a single broadened molecular orbital. The molecular switches exhibit a pronounced hysteretic switching behavior when the bias voltage exceeds a certain value ($\approx 0.4V$).

TT 35.24 Wed 14:00 P1A

Optical Spectroscopy on Tuneable Nano Gaps — •Daniel Gerster[1], Joachim Reichert[1], Stefan Klein[2], Harald Fuchs[2], and Johannes V. Barth[1] — [1]Physik Department, TU München, Germany — [2]Physikalisches Institut, Universität Münster, Germany

Novel techniques to establish tuneable nano gaps designed to act as electrodes for single molecule charge transport measurements are required both for fundamental research and device oriented applications. Hereby, the implementation of additional control parameters to influence the properties of the functional molecule within the gap is of special interest. We present a method to fabricate tuneable nanoscale electrodes where an apertureless scanning nearfield tip (SNOM-tip) is employed to serve as a counter electrode in a molecular junction and simultaneously as a light source. The apertureless SNOM-tip acts as plasmonic waveguide to focus surface plasmon polaritons to the apex of the tip, where a strongly enhanced evanescent field is confined to only a few nanometers. First spectroscopic measurements of light absorption at the empty gap reveal distinct standing wave patterns of optical waves between the electrodes, indicating high field intensities in the gap region.

TT 35.25 Wed 14:00 P1A

Phase-dynamics in superconducting atomic and molecular point contacts — •Benjamin Obert — Institut für theoretische Physik, Universität Ulm, Germany

In the conventional theory for current biased superconducting atomic point contacts the dynamics of the phase difference across the contact is described on single adiabatic surfaces for the Andreev bound states. Here we consider

(i) non-adiabatic transitions between these surfaces relevant for highly transmitting channels and

(ii) energy dependent transmission channels which may occur in molecular junctions.

TT 35.26 Wed 14:00 P1A

Charge transport through an interference SET — •Georg Begemann, Dana Darau, Andrea Donarini, and Milena Grifoni — University of Regensburg, Germany

We study the charge transport through a benzene interference single electron transistor. The interplay between Coulomb interaction and orbital symmetry produces specific transport characteristics that can be considered as the fingerprints of the contacted molecule. Specifically we predict selective conductance suppression and the appearance of negative differential conductance and current blocking when changing the contacts from para to meta configuration[1,2]. All effects originate from destructive interference in transport involving states with orbital degeneracy.

The studied transport phenomena are also robust under the perturbation exerted by the anchor groups binding the contact atoms to the leads or by an external electrostatic field.
[1] G.Begemann, D.Darau, A.Donarini, and M.Grifoni, Phys. Rev. B 77, 201406(R) (2008).
[2] D.Darau, G.Begemann, A.Donarini, M.Grifoni, arXiv:0810.2461

TT 35.27 Wed 14:00 P1A

Electron Dynamics in Molecular Wires Studied by a Density Matrix Approach — •Lisa Mövius and Ulrich Kleinekathöfer — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Recent investigations in the field of molecular electronics [1-3] are targeted on controlling the current through single molecules by laser fields.