can be controlled by *electrochemical gating* [1,2]. Based on density functional theory calculations, we show that molecules under study behave as weakly coupled quantum dots, where the current is carried by a redox-active LUMO-(lowest unoccupied molecular) level [3]. We calculate how the conductance decays with increasing the wire length and thereby recover quantitatively the experimental tunneling exponent [4]. Our calculations imply, that the charging induced conformational change in the bipyridinium unit is not a main switching agent, rather than the phonon-assisted inelastic electron transport through the viologen redox-level explains the observed switching behavior [3].

[1] W. Haiss *et al.*, J. Am. Chem. Soc. **125**, 15294 (2003). [2] Zh. Li *et al.*, Nanotechnology, **18**, 044018 (2007). [3] A. Bagrets, A. Arnold, and F. Evers, arXiv:0711.XXXXv1. [4] Ch. Li, I. Pobelov, Th. Wandlowski, A. Bagrets, A. Arnold, and F. Evers, to appear in J. Am. Chem. Soc.

TT 14.2 Tue 9:45 H 3010

Effects of polaron hopping on the transport through DNA — •Benjamin B. Schmidt[1,2], Matthias H. Hettler[2], and Gerd Schön[1,2] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Postfach 3640, 76021 Karlsruhe, Germany

Experiments probing the equilibrium transport in DNA [1] have led to the consensus that polaron hopping is the dominant transport mechanism of charge carriers in DNA. On the other hand in non-equilibrium experiments where short DNA molecules are connected to two biased leads various types of behaviour is seen (reaching from ballistic transport to insulating behaviour). The reason for this discrepancy is not resolved. We suggest that polaron hopping plays an important role in the non-equilibrium transport through DNA. Our theory is based on work by Böttger and Bryksin [2] on small polaron transport in bulk materials, which we extend to nanostructures where we also account for coupling of the DNA to the leads. It desribes the polaron hopping quantum mechanically by expanding the time evolution of the occupation number on the different bases along the Keldysh contour. We observe non-symmetric current-voltage characteristics which we relate to partial charge redistribution on the DNA due to the applied bias.

[1] P.Henderson et al., PNAS USA, **96**, 8353 (1999)

[2] H. Böttger and V. V. Bryksin, 'Hopping conduction in Solids', Akademie Verlag Berlin, (1985)

TT 14.3 Tue 10:00 H 3010

Dynamical effects in the conductance properties of short DNA molecular wire: a combined study using molecular dynamics and model Hamiltonians — •Rodrigo Caetano[1], Rafael Gutierrez[1], Ben Woiczikowski[2], Tomas Kubar[2], Marcus Elstner[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center for Biomaterials, Dresden University of Technology, D-01062 Dresden, Germany — [2]Institute for Physical and Theoretical Chemistry, Braunschweig University of Technology, D-38106 Braunschweig, Germany

The potential applications of DNA either as template or as molecular wires make of crucial importance to understand the microscopic mechanism leading supporting (or hindering) charge migration through this molecule. The experimental studies give very striking results, which range from insulating up to superconducting behavior. Theoretically, it is very important to include dynamical effects, since DNA is known to be a very flexible molecule. The dynamical effects of the solvent should be taken into account. In this work, we study charge transport through short Poly(G)-Poly(C) DNA within a minimal tight binding model. The model parameters are extracted from snapshots along QM/MM trajectories via DFTB approximation and thus include internal and solvent dynamical effects. We perform a statistical analysis of the time-dependent onsite and electronic hopping and show a broad non symmetric distribution. Green function formalism is used to calculate the transport characteristics and demonstrate how the average quantities depend on the relation between system time scales.

TT 14.4 Tue 10:15 H 3010

Switching response of DNA conduction under stretching — •Bo Song[1], Marcus Elstner[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science, Dresden University of Technology, D-01062 Dresden, Germany — [2]Institute for Physical and Theoretical Chemistry, Braunschweig University of Technology, D-38106 Braunschweig, Germany

By merging DFTB calculations and model-Hamiltonian approaches, we study the stretching-twisting process of poly(GC) DNA oligomers. A local maximum for the transfer integral t between two nearest-neighbor GC pairs is found in the stretching process, which arises from the competition between stretching and twisting. This results in a local maximum for the current in the case that the electrode-DNA coupling Γ is greater than t. Reducing Γ to the values smaller than t gives rise to plateaus in the current. The heights of such plateaus are almost equal to each other.

TT 14.5 Tue 10:30 H 3010

Modeling of tunneling through single endohedral N@C$_{60}$ molecules — •Carsten Timm[1], Jacob E. Grose[2], Wolfgang Harneit[3], and Daniel C. Ralph[2] — [1]University of Kansas, Lawrence, USA — [2]Cornell University, Ithaca, USA — [3]Freie Universität Berlin, Germany

We report on recent experimental and theoretical results for single-molecule transistors involving endohedral N@C$_{60}$ fullerene molecules. In this talk, we will focus on the theoretical modeling. The observed differential conductance shows strong evidence for the exchange interaction between electrons in the fullerene LUMO and the nitrogen p-electrons, favoring an antiferromagnetic interaction. In addition, soft vibrational modes are seen, which are attributed to oscillations of the molecule as a whole. We discuss a model Hamiltonian that reproduces the main features of the experimental conductance.

TT 14.6 Tue 10:45 H 3010

Silicon based nanogap devices for transport studies on molecule-nanoparticle junctions — •Sebastian Strobel[1], Rocio Murcia[1], Allan Hansen[2], and Marc Tornow[2] — [1]Walter Schottky Institut, TU München, Germany — [2]Institut für Halbleitertechnik, TU Braunschweig, Germany

One possible realization of future nanoelectronics may be a hybrid combination of existing silicon circuitry with functional molecular units. Such approach requires a silicon based technology that allows for the parallel fabrication of contact structures for molecules, as well as the fundamental characterization of such hybrids.

We have fabricated arrays of individually addressable nanogap electrodes with a predefined separation down to ˜20 nm using silicon on insulator (SOI) as substrate material. The samples were processed using standard optical lithography, dry and wet chemical etching, and metal thin film deposition, only.

We realized hybrid molecular junctions using such nanogap electrode devices by self-assembling a monolayer of mercaptohexanol onto the metal contacts, and trapping 30 nm diameter Au nanoparticles between the functionalized electrodes, subsequently. Transport measurements at 4.2 K revealed pronounced Coulomb staircase behaviour, characteristic for asymmetric double-barrier tunnelling junctions. We analyse our data by means of model calculations.

TT 14.7 Tue 11:00 H 3010

Length-dependent conductance and thermopower in metal-molecule-metal junctions — •Janne Viljas[1,2], Fabian Pauly[1], and Juan Carlos Cuevas[3,1,2] — [1]Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures, Universität Karlsruhe, D-76128 Karlsruhe — [2]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, D-76021 Karlsruhe — [3]Departamento de Física Teórica de la Materia Condensada C-V, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

Using a method based on density-functional theory, we investigate the conductance and the thermopower in metal-molecule-metal junctions made of dithiolated oligophenylenes contacted to gold electrodes [1]. We find that while the conductance decays exponentially with increasing molecular length, the thermopower increases linearly in good quantitative agreement with recent experiments [2]. We also analyze how these transport properties can be tuned with methyl side groups. The characteristic substituent effects in our ab-initio calculations are explained using a π-electron tight-binding model, which we have studied in detail.

[1] F. Pauly, J. K. Viljas, and J. C. Cuevas, arXiv:0709.3588.

[2] P. Reddy *et al.*, Science **315**, 1568 (2007).

15 min. break

TT 14.8 Tue 11:30 H 3010

Current switching in single molecule transport and con-