TT 40: TR: Nanoelectronics III: Molecular Electronics 2

Time: Friday 10:15–13:45   Location: H20

Invited Talk   TT 40.1   Fri 10:15   H20
Heating, Heat Conduction and Cooling in Molecular Junctions — •ABRAHAM NITZAN[1], MICHAEL GALPERIN[2], and KEIJI SAITO[3] — [1]School of Chemistry, Tel Aviv University, Tel Aviv 69978, Israel — [2]Department of Chemistry, University of California, La Jolla, CA, 92093, USA — [3]Graduate School of Science, University of Tokyo, 113-0033, Japan

Heating in molecular conduction junction depends on the balance between the rate of heat deposit by the electronic current and the efficiency of heat conduction away from the junction. I will review our recent work on such processes, then focus on models for current induced cooling in such systems.

          TT 40.2   Fri 10:45   H20
Spin-polarized transport and thermoelectric properties of organometallic nanocontacts — •STEVEN ACHILLES[1], VOLODYMYR V. MASLYUK[1], MADS BRANDBYGE[2], and INGRID MERTIG[1] — [1]Institute of Physics, Martin Luther University, D-06120 Halle, Germany — [2]DTU Nanotech - Department of Micro- and Nanotechnology, Technical University of Denmark, DK-2800 Kongens Lynby, Denmark

Understanding the electronic and thermoelectric transport properties is the key issue in understanding new devices based on the principles of quantum mechanics. We present a theoretical study of the length dependence of both conductance and thermopower of organometallic vanadium-benzene molecules ($V_n Bz_{n+1}$) sandwiched between magnetic Co(100) electrodes. We show that the molecules with $n \geq 3$ are efficient spin-filters. Namely, we find that the zero bias conductance of the majority electrons is small and decays exponentially with increasing length of the molecule and is in the tunneling regime while the minority electrons show metallic conductance. We show furthermore that the thermopower strongly depends on the length of the molecules and can even change sign as a function of length and temperature [1], and as a function of the relative orientation of the lead magnetizations [2].

[1] V. V. Maslyuk, S.Achilles, and I. Mertig, Solid State Communications, in press
[2] V. V. Maslyuk, S.Achilles, and I. Mertig, submitted

          TT 40.3   Fri 11:15   H20
Single-Molecule Junctions: progress on gated mechanically controlled break junctions — •STEFAN BALLMANN, STEFAN WAGNER, DANIEL SECKER, and HEIKO B. WEBER — Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Staudtstr. 7/A3, D-91058 Erlangen, Germany

The mechanically controlled break junction (MCBJ) technique provides a powerful tool for immobilization of single molecules between two atomically sharp gold tips. However, three-terminal devices incorporating a gate electrode have not been realized on highly flexible substrates so far.

Here we report on promising methods to reproducibly structure an insulating layer in between two metal bridges within a three-step electron beam lithography process. The misalignment of both bridges has been successfully reduced below 25 nm. Moreover, the 15 nm insulating layer is highly stable upon bending the substrate while the leakage current remains below 1 nA at gate voltages of ± 4.5 V. The formation of atomically sharp gold contacts is not perturbed by the presence of the gate. We consider this as an important experimental step towards gated single-molecule contacts.

          TT 40.4   Fri 11:45   H20
Electronic Transport Measurements on Si_4 Clusters — •JOCHEN GREBING[1,2], RAINER DIETSCHE[1], GERD GANTEFÖR[1], THOMAS KIRCHNER[1], and ELKE SCHEER[1] — [1]Department of Physics, University of Konstanz, D-77457 Konstanz, Germany — [2]Forschungszentrum Dresden-Rossendorf, D-01328 Dresden, Germany

A still intriguing issue in the field of molecular electronics is the dependence of the transport properties of a molecule or cluster on the exact geometric realization of the contact at the atomic scale. Here, Si_4 clusters come in handy as they have a very well known rhombohedral geometry as well as a limited yet diverse number of possibilities of being contacted.

After soft-landing from the gas phase, using a mechanically controlled breakjunction technique, possibly single or few Si_4 clusters were contacted with atomically sharp tips and transport characteristics were measured. In addition to conductance histograms, current-voltage (IV) curves with and without clusters in the junction have been recorded. By comparison with the outcome of DFT calculations, the presence of the clusters could be identified in the histograms.

By fitting a resonant tunneling model to the IV curves, the coupling between the clusters and the leads as well as the energy difference of the molecular orbital contributing to the transport and the Fermi energy in the leads could be determined.

We thank F. Pauly for providing the DFT code and for introducing us to it's use, A. Erbe and J. C. Cuevas for the introduction to the resonant tunneling model and valuable discussions.

15 min. break

          TT 40.5   Fri 12:30   H20
Density-functional study of transmission channel degeneracy in biphenyl-based single-molecule junctions — •M. BÜRKLE[1], F. PAULY[1], J.K. VILJAS[1], and G. SCHÖN[1,2] — [1]Institut für Theoretische Festkörperphysik, KIT, 76128 Karlsruhe, Germany — [2]Institut für Nanotechnologie, KIT, 76128 Karlsruhe, Germany

Using density functional theory, we investigate the charge transport for a series of biphenyl molecules [1]. The torsion angle between the two phenyl rings, and hence the degree of π conjugation is controlled by alkyl chains and methyl side groups. Considering different bonding geometries, we find that the conductance can vary by one order of magnitude for the same molecule [2]. We explain this by the different hybridisation of molecular states with those of the electrode. For all molecules, except for those with completely broken conjugation, we observe that the transmission is dominated by one channel, formed from the π electrons. For molecules with D_{2d} point group symmetry at 90°, two degenerate transmission channels should dominate the transport. However, in the molecular junction the electrodes reduce the symmerry and destroy the channel degeneracy. We show that for bonding geometries with a small degree of hybridisation between the electrode and the molecule, nevertheless, the channel degeneracy presists .

[1] A. Mishchenko, D. Vonlanthen, V. Meded, M. Bürkle, C. Li, I.V. Pobelov, A. Bagrets, J.K. Viljas, F. Pauly, F. Evers, M. Mayor, and T. Wandlowski, Nano Lett. (in press).
[2] M. Bürkle, F. Pauly, J.K. Viljas, V. Meded, A. Bagrets, and G. Schön (submitted).

          TT 40.6   Fri 12:45   H20
Vibronic Cooling Mechanisms in Molecular Junctions — •RAINER HÄRTLE[1], MICHAEL THOSS[1], ROIE VOLKOVICH[2], and URI PESKIN[2] — [1]Theoretische Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany — [2]Schulich Faculty of Chemistry, Technion-Israel Institute of Technology, Haifa 32000, Israel

We study vibrational nonequilibrium effects in charge transport through single-molecule junctions. Vibrational degrees of freedom of a molecular junction can be excited by inelastic electron transmission processes (local heating). Such processes are active even if the junction is in its vibrational ground state or thermal equilibrium, and manifest themselves in pronounced structures in the junction's transport characteristics. Cooling processes, however, can usually only occur if the junction is driven out of thermal equilibrium and require the junction to provide vibrational energy. We show that these processes may be as important as heating processes and that local cooling may induce transport phenomena, which are not present in thermal equilibrium. The methodology we have used to study these transport phenomena includes a nonequilibrium Green's function approach [1,2,3], and a master equation approach [3], which provide complementary schemes.

[1] M. Galperin, A. Nitzan, M. A. Ratner, Phys. Rev. B 73, 045314 (2006).
[2] R. Härtle, C. Benesch, M. Thoss, Phys. Rev. B 77, 205314 (2008).
[3] R. Härtle, C. Benesch, M. Thoss, Phys. Rev. Lett. 102, 146801 (2009).

TT 40.7 Fri 13:00 H20

Controlling the conductance of molecular wires by defect engineering: a *divide et impera* approach — ●Daijiro Nozaki[1], Horacio M. Pastawski[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, Dresden, Germany — [2]Instituto de Física Enrique Gaviola (CONICET) and Facultad de Matemática, Astronomía y Física, Universidad Nacional de Córdoba, Córdoba, Argentina

Charge transport through 1D molecular systems connected between two contacts is influenced by several parameters such as the electronic structure of the molecule and the presence of disorder and defects. In this work, we have modeled 1D molecular wires connected between electrodes and systematically investigated the influence of both soliton formation and the presence of defects on properties such as the conductance and the density of states. Our numerical calculations have shown that the transport properties are highly sensitive to the position of both solitons and defects. Interestingly, the introduction of a single defect in the molecular wire which divides it into two fragments both consisting of an odd number of sites creates a new conduction channel in the center of the band gap resulting in higher zero-bias conductance than for defect free systems. This phenomenon suggests routes toward engineering molecular wires with enhanced conductance.

TT 40.8 Fri 13:15 H20

Electron transport through σ- and π-derived transmission channels — ●Shigeru Tsukamoto, Vasile Caciuc, Nicolae Atodiresei, and Stefan Blügel — Institut für Festkörperforschung & Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

Nanoscale electronic devices utilizing organic molecules, a possibility that was revealed in the 1970's, have been ceaselessly studied experimentally and theoretically. Nowadays, various organic molecules are recognized as potentially functional components for future molecular devices. In some molecules, the functionality may rely on the difference in electron transport properties between the σ and π states.

In this paper, we theoretically investigate the electron transport through σ- and π-derived transmission channels of organic molecules, and discuss the difference in transport properties between them. Transport calculations are carried out by means of the Lippmann-Schwinger equation and a real-space finite-difference method based on the density functional theory (DFT).

As a preliminary calculation, we have investigated the transport property of a benzene molecule sandwiched between a pair of planar metal electrodes, which involves both σ and π states. Although no electron transport through any of the two transmission channels are confirmed at the Fermi level, significant electron transmission through a π-derived channel can be seen at 0.7eV above the Fermi level. In the presentation, we are going to show electron transport properties of larger molecules followed by detailed discussions on the functionality.

TT 40.9 Fri 13:30 H20

Dynamical properties of charge transport in organic systems — ●Pedro D Manrique[1,2], Rafael Gutierrez[1], Gotthard Seifert[2], and Gianaurelio Cuniberti[1] — [1]Institute Material Science and Max Bergmann Center of Biomaterials. Dresden University of Technology, Dresden, Germany — [2]Institute of Physical Chemistry and Electrochemistry. Dresden University of Technology, Dresden, Germany

We derive a non Markovian master equation for electronic transport including the interaction with external bosonic degrees of freedom. Within this formalism we calculate the time dependent current (TDC) at different temperatures. Results for the TDC are shown for different values of the coupling to the bosonic environment and we found significant changes in the short-time dynamics. The electronic parameters of the model are calculated via a combination of molecular dynamics simulations with a density functional-based approach including dispersion energy corrections.