TT 44: Transport: Nanoelectronics III - Molecular Electronics 2

Time: Thursday 15:00–17:15 Location: BH 334

TT 44.1 Thu 15:00 BH 334

Charge transport in single molecule junctions with graphene leads — •Ivan Pshenichnyuk, Susanne Leitherer, Pedro B. Coto, and Michael Thoss — Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

High electron mobility, mechanical rigidity and optical transparency make graphene a promising candidate as material for electrodes in nanoelectronic devices. In this work, we investigate charge transport in single molecule junctions with graphene leads. The methodology used is based on a combination of first-principles electronic structure calculations to characterize the molecule-graphene junctions and the Landauer transport formalism. Considering different examples for molecular bridges between graphene electrodes, in particular pentacene-based molecules as well as polyyne chains, we analyze the transmission probability and the current-voltage characteristics.

TT 44.2 Thu 15:15 BH 334

Thermopower of biphenyl-based single-molecule junctions — •Marius Bürkle[1], Linda A. Zotti[2], Janne K. Viljas[3], Thomas Wandlowski[4], Marcel Mayor[5], Gerd Schön[1], and Fabian Pauly[1] — [1]Institut für Theoretische Festkörperphysik and DFG Center for Functional Nanostructures, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain — [3]Low Temperature Laboratory, Aalto University, Aalto, Finland — [4]Department of Chemistry and Biochemistry, University of Bern, Bern, Switzerland — [5]Department of Chemistry, University of Basel, Basel, Switzerland

Employing ab initio electronic structure calculations combined with non-equilibrium Green's function techniques we study the dependence of the thermopower on the degree of π-conjugation in biphenyl-based single molecule gold junctions. We control the degree of π-conjugation by changing the torsion angle φ between the two phenyl rings by means of alkyl side chains connected to the molecules. We find that the absolute value of the thermopower decreases weakly as $\cos^2 \varphi$. We show that the observed $\cos^2 \varphi$ dependence is robust with respect to different anchoring groups and binding positions. The anchoring group determines the sign of the thermopower. Sulfur and amine give rise to $Q > 0$ and cyano to $Q < 0$ respectively. Different binding positions on the contrary lead to variations of the absolute values of the thermopower. The observed ab initio results are found to be described well by means of a π-electron tight binding model.

TT 44.3 Thu 15:30 BH 334

Spin transport and tunable Gilbert damping in a single-molecule magnet — •Milena Filipovic[1], Federica Haupt[2], Cecilia Holmqvist[1], and Wolfgang Belzig[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Institut für Theorie der Statistischen Physik, RWTH Aachen, D-52056 Aachen, Germany

We study spin transport through a molecular level coupled to two leads and a single-molecule magnet in a magnetic field. The molecular spin is treated as a classical variable and, due to the external magnetic field, precesses around the field axis. Expressions for charge and spin currents are derived by means of the Keldysh nonequilibrium Green's function technique in linear response. The exchange coupling between the electronic spins and the magnetization dynamics of the molecule creates inelastic tunneling processes which contribute to the spin currents. The inelastic spin currents, in turn, generate a spin transfer torque [1,2] acting on the molecular spin. This back-action includes one component that gives a contribution to the Gilbert damping and one component that changes the precession frequency. The Gilbert damping coefficient, α, can be controlled by changing the bias and gate voltages, and has a non-monotonic dependence on the tunneling rates. We compare our results to the Gilbert damping coefficient calculated in Ref. [3] in the small precession frequency regime $\hbar\omega \ll k_B T$.
[1] Y. Tserkovnyak et al., Rev. Mod. Phys. 77, 1375 (2005).
[2] C. Holmqvist et al., Phys. Rev. B 83, 104521 (2011).
[3] N. Bode et al., arXiv:1110.4270v1 (2011).

TT 44.4 Thu 15:45 BH 334

THz torsional vibrations in biphenyl-based molecular junc-

tions: transient oscillations and resonance — •Matthias Hinreiner[1], Dmitry Ryndyk[1], Denis Usvyat[2], Thomas Merz[2], Martin Schütz[2], and Klaus Richter[1] — [1]Institute for Theoretical Physics, University of Regensburg, Regensburg, Germany — [2]Institute for Physical and Theoretical Chemistry, University of Regensburg, Regensburg, Germany

We investigate the torsional vibrations in biphenyl-based molecular junctions and transport properties in presence of an external THz field.

Ab-initio calculations with external electric fields show that the torsional angle ϕ of 4,4'-dithiol-biphenyl demonstrates only very tiny response. However, if functional groups are added to the molecule to induce a dipole moment in each of the rings, an external field can change ϕ. Two examples of such molecules are 3,3'-diflouride-4,4'-dithiol-biphenyl and 2,2'-dithiol-5,5'-bipyridine. As the conductivity of biphenyl-based molecules is proportional to $cos^2(\phi)$, we show that the current through these molecules drops if the external THz field frequency gets in resonance to the torsional vibration mode.

15 min. break.

TT 44.5 Thu 16:15 BH 334

Electron transport through helical, biimidazole-based structures — •Thomas Brumme, Rafael Gutiérrez, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany

Molecular electronics and spintronics provide a promising strategy to overcome limitations of semiconductor-based technologies by implementing electronic functionalities at the molecular scale. However, in order to create single molecule spintronics devices one needs to understand the spin-dependent transport through the molecular system, its dependence on different molecular properties and possible mechanisms to change the magnetization of the molecule. Molecular systems with screw symmetry like DNA are especially interesting for spintronics applications since the transport through these systems can be spin selective [1]. We investigate the eletronic structure of a molecular helix formed by silver atoms and biimidazole units ($[Ag(NO_3)(H_2\mathrm{biim})]_n$, [2, 3]). First-principles calculations reveal that several molecular orbitals possess screw symmetry and are completely delocalized along the helix. Based on this results we explore the possibility of spin-selective electron transport through this molecular helix.
[1] B. Göhler et al., Science 331, 894 (2011)
[2] C.A. Hester et al., Polyhedron 16, 2893 (1997)
[3] M. Sowwan et al., Journal of Nanomaterials 2010 (2010)

TT 44.6 Thu 16:30 BH 334

Spin selective transport through helical molecular systems — •Rafael Gutierrez[1], Elena Diaz[2], Ron Naaman[3], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science, Dresden University of Technology, 01062 Dresden, Germany — [2]GISC, Departamento de Fisica de Materiales, Universidad Complutense, E-28040 Madrid, Spain — [3]Department of Chemical Physics, Weizmann Institute, 76100 Rehovot, Israel

Highly spin selective transport of electrons through a helically shaped electrostatic potential is demonstrated in the frame of a minimal model approach. The effect is significant even in the case of weak spin-orbit coupling. Two main factors determine the selectivity, an unconventional Rashba-like spin-orbit interaction, reflecting the helical symmetry of the system, and a weakly dispersive electronic band of the helical system. The weak electronic coupling, associated with the small dispersion, leads to a low mobility of the charges in the system and allows even weak spin-orbit interactions to be effective. The results are expected to be generic for chiral molecular systems displaying low spin-orbit coupling and low conductivity.

TT 44.7 Thu 16:45 BH 334

Quantum Interference Effects in Single-Molecule Junctions — •Stefan Ballmann[1], Rainer Härtle[2], Pedro Brana-Coto[2], Michael Thoss[2], and Heiko B. Weber[1] — [1]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Germany — [2]Institut für Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Germany

We analyze quantum interference effects in single-molecule junctions

both experimentally and theoretically by means of the mechanically controlled break junction technique, density-functional theory and a non-equilibrium Green's function approach. Interference occurs as a suppression of the current level, when quasi-degenerate electronic states contribute to transport. Such levels are quite common in many molecules used for single-molecule junctions. However, such destructive interference can be lifted by coupling the electron system to vibrations, resulting in an enhancement of the current [1]. We demonstrate that this effect is dominant in single-molecule junctions by analyzing temperature dependent IV characteristics.

[1] R. Härtle, M. Butzin, O. Rubio-Pons, M. Thoss, Phys. Rev. Lett. 107, 046802 (2011).

TT 44.8 Thu 17:00 BH 334

STM transport theory for π-conjugated molecules on thin insulating films — •Sandra Sobczyk, Andrea Donarini, and Milena Grifoni — Institute of Theoretical Physics, University of Regensburg, Germany

In seminal experiments, scanning tunneling microscopy (STM) has been performed on molecules on insulating films having a thickness of only few atomic layers. The layer is in turn grown on top of a metallic surface. At the same time the electrons can still tunnel through the insulating films, facilitating spectroscopy and imaging with low-temperature STM.

We present an STM theory that is sufficiently general to be applied to any STM device consisting of a π-conjugated molecule weakly coupled to the substrate and the tip. We show that the strongly asymmetric coupling to the leads, that is provided by the geometry of the substrate and the tip, leads to qualitatively different, energy dependent transfer rates. We apply the theory to a benzene molecule and we demonstrate that the mentioned differences in the rates yield two different types of current suppression, one caused by Coulomb interaction and one by interference effects due to involved orbitally degenerate states. We also simulate constant height current maps and identify the characteristic topographic fingerprints of the two forementioned blocking mechanisms.