TT 21: TR: Nanoelectronics III - Molecular Electronics 2

Time: Tuesday 10:30–13:00 Location: HSZ 301

TT 21.1 Tue 10:30 HSZ 301

Spatio-Temporal description of Quantum Transport — •Björn Oetzel[1,2], Friedhelm Bechstedt[1,2], and Karsten Hannewald[1,2] — [1]Institut für Festkörpertheorie 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 method for the calculation of time-dependent transport properties of non-periodic systems connected to electron reservoirs. The approach is based on the solution of the time-dependent Schrödinger equation combined with the emitting boundary conditions using plane waves as modeling of the leads.

Using the approach we are able to simulate the temporal evolution of wave packets through potential barriers. Within the quasi-stationary limit the method can be associated with the Landauer Formalism. Transmission functions are calculated directly from the transmitted and reflected currents for the insertion of a single plane wave. Beyond the calculation of transmission functions the approach is also capable of field-dependent transport properties such as current voltage characteristics. Those can be calculated independently of the transmission functions including by direct treatment of time-dependent potentials and electrical fields, in contrast to the Landauer approach. The success of the method is demonstrated by 1D-model calculations for single and double barriers including modifications due to applied electrical fields.

TT 21.2 Tue 10:45 HSZ 301

Highly controllable fabrication of horizontally aligned single walled carbon nanotubes — •Imad Ibrahim[1,2], Alicja Bachmatiuk[2], Jan Blüher[1], Felix Börrnert[2], Mark H. Rümmeli[2,3], Bernd Büchner[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science, TU-Dresden, 01062 Dresden, Germany — [2]Institute for Solid State Research, IFW Dresden, 01171 Dresden, Germany — [3]Department of Physics, TU-Dresden, 01062 Dresden, Germany

Single-walled carbon nanotubes (SWCNTs) are considered a promising material for future nanoelectronics because of their excellent electronic and physical properties. Their electronic properties strongly depend on their diameter and chiral angle. SWCNTs are divided into metallic and semiconductor SWCNTs. High yield semiconductor horizontally well-aligned SWCNT are essential for molecular electronics applications, in which one needs to fabricate parallel active devices, such as diodes and transistors. In this study, well-defined protocols have been developed for growing horizontally well-aligned carbon nanotubes in high yield via chemical vapor deposition. The developed route provides a high degree of control of various aspects, such as the tube length, yield, quality and the alignment of the tubes. The as-grown CNT are characterized with different techniques; scanning electron microscopy, atomic force microscopy, Raman spectroscopy and transmission electron microscopy.

TT 21.3 Tue 11:00 HSZ 301

Interference and transport through π-conjugated molecules in an STM set-up — •Sandra Kolmeder, Andrea Donarini, and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg

We develop a general STM transport theory for π-conjugated molecules, based on the density matrix formalism. The focus is on STM experiments which measure electronic properties of individual molecules deposited on ultra-thin insulating films on metal substrates, where the insulating film allows to electronically decouple the molecule from the metallic surface. We model this geometry as a double-barrier tunneling set-up where we account for angular momentum selection rules governing tunneling processes from the tip to the molecule and from the molecule to the substrate. Applied to a benzene molecule we find that angular momentum conservation rules allow to express the STM tunneling current in terms of few relevant "angular momentum channels". In the tunneling the molecule changes free energy F and angular momentum l. In turn the tunneling rate changes of several orders of magnitude depending on ΔF and Δl. We will show that current blocking occurs as an interference effect, because of involved orbitally degenerate states.

TT 21.4 Tue 11:15 HSZ 301

Electron transport through π-conjugated molecules anchored via carboxilate groups to Cu(110) electrodes — •Shigeru Tsukamoto, Vasile Caciuc, Nicolae Atodiresei, and Stefan Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Nowadays, carboxilate-Cu bonds[1] are recognized as an alternative to the thiolate-Au bonds to be used in future molecular electronic devices. As a consequence, a clear understanding of the electron transport properties is highly desirable and, in particular, *ab initio* simulations are used to elucidate and design the functionality of specific molecules in a given organic-metal electrode environment.

Here we report on the transmission properties of three aromatic molecules anchored via carboxyliate groups to the Cu(110) electrodes. In our approach, the scattering wave functions are computed by solving the Lippmann-Schwinger equation.

While thiolate-Au systems show both sharp and broad transmissions peaks, the electron transmissions of the aromatic carboxilates-Cu molecular systems exhibit only sharp peaks. This implies that the molecular system with carboxilate-Cu bonds are more sensitive to change in bias voltage as compared to that with thiolate-Au ones. Furthermore, we demonstrate that the switching property of the molecules can be locally controlled by replacing a CH group of the aromatic ring with an N atom since the transmissions peaks are shifted to lower energies keeping the peak-peak distance.

[1] M. C. Lennartz *et al.*, Langmuir, **25**, 856 (2009).

TT 21.5 Tue 11:30 HSZ 301

Conformational changes in biphenyl under applied voltage — •Lars Kecke and Joachim Ankerhold — Institut für theoretische Physik, Universität Ulm

The usual way to calculate the transmission of a molecule is to calculate the transmission matrix of an isolated molecule and then to add the leads. We show that, especially in case of molecules with intrinsic switching probabilities, this procedure leads to massively incorrect conductivities. We have used a Born-Oppenheimer-like master-equation approach to calculate the energy profile of the torsional degree of freedom in a molecule of biphenyl in the presence of two electrodes and found the torsional angle snapping from a roughly 45-degree position at low voltage to zero, accompied by a quantization of current, in a pattern reminiscent of Coulomb diamonds.

15 min. break

TT 21.6 Tue 12:00 HSZ 301

Coherent transport and the effects of strong correlations in cobalt-benzene sandwich molecules — •Michael Karolak[1], David Jacob[2], and Alexander Lichtenstein[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

We study the impact of dynamical correlations on the electronic structure and coherent transport properties of cobalt-benzene sandwich molecules (see e.g. [1]) hosted in a copper nanocontact. The interactions of the Co 3d electrons are fully taken into account by combining density functional calculations with a dynamical treatment of the strong correlations in the Co 3d shell in the one-crossing approximation [2]. We find that depending on the geometry of the contact region the hybridization of the Co 3d shell with the benzene ring states and dynamical correlations give rise to the Kondo effect and thus lead to Fano-like features in the coherent transport characteristics.

[1] T. Kurikawa et al. J. Phys. Chem. 99, 16248 (1995)
[2] D. Jacob et al. Phys. Rev. Lett. 103, 016803 (2009)

TT 21.7 Tue 12:15 HSZ 301

Ab initio Anderson-Hubbard model of molecular junctions — •Dmitry Ryndyk and Klaus Richter — Institute for Theoretical Physics, University of Regensburg, Regensburg, Germany

Electron-electron interaction plays an important role in transport through single-molecule junctions, controlling a position of resonant levels and leading to Coulomb blockade and Kondo effect in the case of weak coupling to the leads. The methods of many-body theory

are necessary to explain nonequilibrium correlation effects. On the other hand ab initio approach is required to take into account realistic geometry and electronic structure of molecular junctions. The task of modern theory is to combine ab initio and many-body quantum transport methods. We developed a theoretical approach to describe single-molecule junctions in terms of Anderson-Hubbard Hamiltonian in the basis of localized molecular orbitals. The matrix elements of the effective Hamiltonian are calculated by GAMESS and Firefly (former PC GAMESS) quantum chemistry codes. The transport at finite voltage is described in the framework of nonequilibrium Green function or generalized master equation approaches. The systems, to which we apply the method, include oligophenyl (benzene, biphenyl, terphenyl an other) junctions and metal-phtalocyanines.

TT 21.8 Tue 12:30 HSZ 301

How Vibrations Generate Electrical Current: Decoherence in Single-Molecule Junctions — •Rainer Härtle, Michael Butzin, and Michael Thoss — Theoretische Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany

Employing a nonequilibrium Green's function approach [1,2], we analyze quantum interference effects and decoherence mechanisms in single-molecule junctions. Quantum interference effects have been found to be of importance in coherent electron transport for different types of nanostructures [3,4], in particular for single-molecule junctions [5]. These effects may result in a suppression of the electrical current due to destructive interference. In the presence of electronic-vibrational coupling, however, this suppression may not fully develop or completely disappears, especially if the vibrational degrees of freedom are highly excited. This is demonstrated for a generic model system and for a realistic model of a biphenyl-acetylene-dithiolate molecular junction, where strong dephasing results from a multitude of vibrational modes. The currents are significantly larger than without electronic-vibrational coupling. In other words, vibrations generate electrical current by quenching of desctructive interference.

[1] R. Härtle *et al.*, Phys. Rev. B 77, 205314 (2008).
[2] R. Härtle *et al.*, Phys. Rev. Lett. 102, 146801 (2009).
[3] B. Kubala, J. König, Phys. Rev. B 65, 245301 (2002).
[4] A. Donarini *et al.*, Phys. Rev. B 82, 125451 (2010).
[5] G. C. Solomon *et al.*, Nano Lett. 6, 2431 (2006).

TT 21.9 Tue 12:45 HSZ 301

Vibration-assisted tunneling through a molecular level with competing phonon modes — •Federica Haupt[1,2], Johannes Buelte[1], and Wolfgang Belzig[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Institut für Theoretische Physik A, RWTH Aachen, D-52074 Aachen, Germany

We investigate the electronic transport properties of a single electronic level weakly coupled to leads and interacting with two different phonon modes. We consider the interplay between the two phonon modes under the assumption that tunneling induces a non–equilibrium vibrational distribution and compare to the opposite limit of strong relaxation of the vibrations due to some dissipative environment. We show that in the presence of non–equilibrium the tunneling electrons mediate an effective interaction between the two phonon modes. This results in characteristic features in the transport properties of the device such as sub-threshold excitation of one phonon mode and the appearance of negative differential conductance in a wide range of parameters.