TT 32.9 Di 18:15 TU H2053

Strong Coulomb effects in hole-doped Heisenberg chains — •Jürgen Schnack — Universität Osnabrück, Fachbereich Physik, D-49069 Osnabrück, Germany

Substances like the "telephone number compound" $Sr_{14}Cu_{24}O_{41}$ are intrinsically hole-doped. The involved interplay of spin and charge dynamics is a challenge for theory. In this Letter we propose to describe hole-doped Heisenberg spin rings by means of complete numerical diagonalization of a Heisenberg Hamiltonian that depends parametrically on hole positions and includes the screened Coulomb interaction among the holes. It is demonstrated that key observables like magnetic susceptibility, specific heat, and inelastic neutron scattering cross section depend sensitively on the dielectric constant of the screened Coulomb potential which opens the fascinating possibility to determine the in-medium dielectric constant experimentally from such observables [1,2].
[1] J. Schnack, Phys. Rev. Lett., submitted, cond-mat/0409650
[2] J. Schnack, F. Ouchni, J. Magn. Magn. Mater. (2004) accepted, cond-mat/0406592

TT 33 Transport - Nanoelectronics III: Molecular Electronics

Zeit: Dienstag 14:00–18:00 Raum: TU H3027

TT 33.1 Di 14:00 TU H3027

A single-molecule diode — Rolf Ochs[1], Mark Elbing[1], Marcel Mayor[1], Max Köntopp[1], Ferdinand Evers[1], and •Heiko B. Weber[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Postfach 3640, D-76021 Karlsruhe — [2]Institut für Angewandte Physik, Universität Erlangen, Staudtstr. 7, 91058 Erlangen

We have designed and synthesized an organic molecule such that it can be used as a diode on the single-molecule level. Individual molecules were contacted employing the mechanically controlled break junction technique. The results show indeed diode-like current-voltage characteristics. In contrast to that, control experiments with similar symmetric molecules did not show significant asymmetries in the transport properties. In order to investigate the underlying transport mechanism, phenomenological arguments are combined with calculations based on density functional theory. It turns out that the physics responsible for the asymmetry has several analogies to that in a p-n semiconductor diode.

TT 33.2 Di 14:15 TU H3027

Electrical transport through DNA molecules under stretching — •Ning Kang, Roman Lehner, Artur Erbe, and Elke Scheer — Department of Physics, University of Konstanz, Germany

Understanding the mechanism of electron motion along DNA is an essential step for the development of DNA-based molecular electronics. However, a number of contradicting findings were reported regarding the electronic properties of DNA. Theoretical calculations have demonstrated that the charge transport through the DNA will be strongly influenced by conformational transitions. To probe this effect, we have measured the resistance of DNA molecules under stretching with the help of the mechanically controllable break junction technique (MCB). Using the break junctions, we are able to fabricate electrodes with nanometer separation and fine-tune the tunneling gap between electrodes down to a resolution in the picometer range. In our experiments, we used 10-nm-long (30 base pairs) DNA with thiol groups at both ends, and stretched continuously the trapped molecules by means of MCB. A discrete two-level resistance switching behavior is observed when changing the distance of the electrodes, which might be related to a conformation transition of the DNA under stretching. To clarify whether the measured signal is from molecules, we also perform the measurements with a specific enzyme that cuts the DNA.

TT 33.3 Di 14:30 TU H3027

Dissipative Effects in the Electronic Transport through DNA molecular wires — •Rafael Gutierrez, Sudeep Mandal, and Gianaurelio Cuniberti — Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg

DNA-based molecular wires have a huge potential for application in molecular electronics. Their electronic transport properties are however not well elucidated. This is mainly due to the extreme sensitivity of charge propagation in DNA to static and dynamic disorder as well as to environmental effects (counterions, water shell, etc). We investigate the influence of a dissipative environment which effectively comprises the effects of counterions and hydration shells, on the transport properties of short DNA wires. For this purpose we use a tight-binding model embedded in a bosonic bath consisting of a collection of harmonic oscillators. In the absence of interactions with the bath, a temperature independent gap opens in the electronic spectrum. Upon allowing for electron-bath coupling the gap becomes temperature dependent. We show that a crossover from semiconducting to metallic behavior in the low-voltage region of the I-V characteristics can be achieved in some parameter regions. The reason is the appearance of bath-induced polaronic states within the electronic bandgap. We further show that the temperature dependence of the transmission near the Fermi energy displays an Arrhenius-like behavior in agreement with recent transport experiments.

TT 33.4 Di 14:45 TU H3027

Characterization of nanoscale molecular junctions — •Artur Erbe[1], Anat de Picciotto[2], Jennifer E. Klare[2], Colin Nuckolls[2], Kirk Baldwin[3], and Robert Willett[3] — [1]Universität Konstanz, FB Phyisk — [2]Columbia University, NY, USA — [3]Lucent Technologies, Bell Labs, NJ, USA

Exploring the electronic possibilities of nanoscale organic materials has become an important challenge as modern lithographical techniques approach ultimate limits. In this regime, the properties of single or a few molecules will dominate the behavior of whole devices. Recent experiments on nanoscale molecular junctions show a large variety of results. Differences in the properties of the molecules themselves cannot fully account for these variations. This fact indicates that contact properties play an important role in the behavior of the whole junction. We present electrical measurements of various types of molecules using an electrical break junction technique. The formation of the junctions relies on electromigration in a narrow gold wire. This technique allows us to test the junctions under varying external conditions. Distinct features are found in the I-V-characteristics at low temperatures indicating that single or a few molecules are contacted. Some of those features can be affected by changes in applied gate voltage. The energy scales associated with these features cannot be explained with molecular properties alone. In order to explain our results we take interactions between the molecules and the contacting metals into account.

TT 33.5 Di 15:00 TU H3027

Electron-phonon interactions in atomic-scale conductors — •Janne Viljas, Fabian Pauly, and Juan Carlos Cuevas — Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe

With the recent advances in nanofabrication techniques it has become possible to manipulate and explore the electronic transport through atomic-scale wires and individual molecules. This has posed an exciting theoretical challenge, namely the understanding of the conduction mechanisms at the molecular scale. So far, the effort has been mostly concentrated on analysing the role of the electronic structure of the atomic-scale conductors, but little has been done on the role of their internal degrees of freedom. In this talk I will present our efforts to understand what are the effects of the vibrational modes on conduction at the atomic scale. In particular, making use of a tight-binding approach, we describe the influence of the inelastic electron-phonon processes in metallic atomic wires. This allows us to address many different questions such as (i) what determines that in some experimental situations the vibrational modes enhance the current and in some others they reduce it? (ii) What are the possible signatures of these modes in the current-voltage characteristics? (iii) What are the selection rules that explain why some vibrational modes do not show up in the transport experiments?

TT 33.6 Di 15:15 TU H3027

Electron-phonon coupling mechanisms in molecular electron transport — •Michael Hartung and Gianaurelio Cuniberti — Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

We study the conductance through a single vibrating molecule contacted to two metallic electrodes. The starting point is a tight-binding Hamiltonian with a linear coupling of the ionic motion to the electronic