quantization or of existence of exceptionally stable radii.

TT 26.30 Wed 14:30 P1

Absence of fractional conductance quantization in ferromagnetic atomic contacts — •Michael Häfner[1], Juan-Carlos Cuevas[1,2,3], Janne Viljas[1], Diego Frustaglia[3], and Fabian Pauly[1] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]Departamento de Física Teórica de la Materia Condensada C-V, Universidad Autónoma de Madrid, 28049 Madrid, Spain — [3]Quantum Transport and Information, Scuola Normale Superiore, 56126 Pisa, Italy

In this work we present a theoretical analysis of the current through atomic contacts of ferromagnetic materials (Co and Ni). Several experimental groups have recently reported the observation of half-integer conductance quantization in nanowires of these materials. This suggests that the current in these contacts is completely spin polarized and all the contributing channels are perfectly transmissive. In order to analyze these surprising observations, we have performed conductance calculations of Ni and Co atomic junctions based on a tight-binding model. Contrary to these experiments, we find that the conductance is in general neither quantized nor spin polarized. We show that the transport is mainly dominated by both the s and d bands close to the Fermi energy. These bands give rise to several conduction channels that are partially open. Typically, both spin bands give a significant contribution to the transport suggesting that the fractional conductance quantization should not appear in ferromagnetic atomic contacts.

TT 26.31 Wed 14:30 P1

Influence of vibrations on electronic transport through DNA — •Benjamin Schmidt[1,2], Matthias Hettler[2], Gerd Schön[1,2], E.B. Starikov[2], and Wolfgang Wenzel[2] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany

Conductance measurements on DNA 'wires' display various types of behavior ranging from insulating over semi-conducting to quasi-metallic, depending on the measurement setup and the measured DNA molecule. The variance of the experimental results as well as ab-initio calculations suggest that the environment and vibrational modes of DNA have a dominating influence on the transport properties of DNA wires. In this work we study transport through simple models of homogeneous DNA wires (poly-DNA) using standard Green function technique and Landauer-Buettiker formalism. In particular, we address the influence of specific DNA vibrational modes (with parameters determined by ab-initio methods) on transport in the presence of an environment described by a general bosonic bath. We can describe the crossover from semi-conducting to quasi-metallic behavior in dependence of temperature and the electronic coupling to the vibrational modes and bath.

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Influence of Adsorbates on the Structure and Electronic Properties of Molecular-size Junctions — •Sören Wohlthat[1], Fabian Pauly[1], Janne Viljas[1], Juan-Carlos Cuevas[2,1,3], and Gerd Schön[1,3] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe — [2]Departamento de Física Teórica de la Materia Condensada C-V, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [3]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe

During the last few years, the conduction properties of molecuar-size contacts between two metallic leads have attracted a great deal of attention. Motivated by recent experiments concerning the effect of hydrogen [1] and oxygen [2] on metallic nanocontacts, we investigate theoretically the influence of adsorbates on this type of junctions. We analyse the stability of different geometries and determine their electronic transport properties. The calculations are based on density functional theory (DFT) using the quantum chemistry package TURBOMOLE. The electronic transport properties are obtained by non-equilibrium Green's function (NEGF) techniques. Our simulations show that adsorbates have a significant influence on the properties of our molecular-size junctions and that they could serve as design tools for future atomic and molecular circuits.

[1] R.H.M. Smit et al., Nature 419, 906, (2002).
[2] W.H.A. Thijssen et al., cond-mat/0509376.

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First-principles study of single row Al and Pt wires — •Thomas Gnielka[1,2], Klaus-Peter Bohnen[1], and Rolf Heid[1] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe — [2]Universität Karlsruhe, Fakultät für Physik, D-76128 Karlsruhe

Over the past several years there has been a great deal of interest in the physical properties of atomic wires. Although there have been some studies of the structural and electronic properties of nanowires so far lattice dynamics of these systems has been hardly studied. This is in strong contrast to the importance of lattice dynamics for structural stability (Peierls transition) and superconductivity. Thus we have investigated the lattice dynamics, the atomic and electronic structures and the relation between them for single-row Al and Pt wires using density-functional theory. The calculations reveal that the wires transform from planar zigzag structure to linear and further to dimerized wires during elongation. Phonon dispersions have been calculated and anomalies nicely correlate with Fermi surface nesting effects. Dimerization effects as seen for Pt wires on Ge(100) seem to be qualitatively in agreement with these findings, however the substrate influence has still to be studied. Prelimenary results seem to indicate the importance of substrate effects.

TT 26.34 Wed 14:30 P1

Transport properties of carbon nanotubes synthesized by chemical vapor deposition — •T. Pietsch, I. Mönch, J. Schumann, K. Biedermann, H. Vinzelberg, and B. Büchner — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

The electrical properties of multiwalled carbon nanotubes (MWCNT) synthesized by chemical vapor deposition (CVD) depend on the used CVD method. In this work we investigate MWCNT with outer diameters from 30 to 60 nm and length over 6 μm grown by a thermal-catalytic CVD method. TEM images show that the concentric layers of the nanotubes are not perfect. The MWCNT devices for the transport measurement with low ohmic contacts were prepared by using an ac-electrophoresis deposition either on Ti-microfinger structures followed by a HV annealing at 800°C or on oxidized silicon wafers with prestructured leads, electron beam lithography, oxygen plasma treatment and evaporated Cr/Au contacts on the nanotubes. The contact resistance are for the Ti contacts about 50 kΩ and for the Cr/Au contacts smaller than 1 kΩ. The average intrinsic room temperature resistance of the MWCNT measured in four-point configuration is 1500 $\mu\Omega$cm and comparable to that of natural graphite of 1350 $\mu\Omega$cm. At room temperature the current-voltage characteristics are linear but at low temperatures not linear. The temperature coefficient of the zero-bias resistance in the temperature range between 300K and 4.2K is negative. Positive magnetoresistances at 4.2K of about 2 % at 8T were measured. The results show that - caused by the defect structure of the MWCNT walls - the conduction is diffusive.

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Transport through molecules — •Bernd Briechle, Simon Verleger, and Artur Erbe — Universität Konstanz, Fachbereich Physik, 78457 Konstanz

The aim of our studies is the characterisation of electronic transport through a single or a few molecules. It is important that the coupling of the molecules to the electrodes is mechanically and electronically stable throughout the experiment. As a first step two different structures allowing for the change of the mechanical coupling will be analysed to find an optimal configuration. On the one hand a mechanically controllable break-junction (MCB) technique will be studied, on the other a shadow evaporation technique based on a silicon structure will be tested. Transport through the molecules can be investigated at different temperatures. Additionally the integration of a gate electrode for detailed characterisation of the charge transport is in preparation.

TT 26.36 Wed 14:30 P1

Hofstadter butterfly of carbon nanotubes — •Norbert Nemec and Gianaurelio Cuniberti — Institut für theoretische Physik, Universität Regensburg, 93040 Regensburg

The electronic spectrum of a two dimensional square lattice in a perpendicular magnetic field, known as Hofstadter butterfly, was discovered in Regensburg thirty years ago [1]. We have calculated the Hofstadter butterfly for carbon nanotubes (CNTs) in the tight-binding approximation. For the case of single wall CNTs, it is straightforward to imple-