degrees of freedom. We distinguish between a coupling to the *onsite* energy of the molecule and a coupling representing a *bond-stretching* vibrational mode.

The full nonequilibrium current, shot noise, and dissipated power is calculated within the Keldysh Green function formalism. As far as transport observables are concerned, onsite and bond-stretching coupling mechanisms differ in several respects: In the latter case satellite peaks in the differential conductance are more pronounced and results closer to the experimental evidence can be obtained.

TT 33.7 Di 15:30 TU H3027

Vibrational effects in transport through a few level molecule. — •Dmitri Ryndyk — Universität Regensburg

We consider a simple molecule with several electron levels placed between large metallic leads. At finite voltage internal vibrations of the molecule as well as an oscillation of the whole molecule between the leads can be excited. We use the self-consistent nonequilibrium theory to describe electron transport through a molecule and dynamics of vibrations. At small voltage or high temperature current is affected by thermally excited vibrations. At larger voltage and low enough temperature transition into the regime with nonequilibrium vibrations is possible. Phase diagram of the system is controlled by coupling to the leads, electron-vibron coupling, and coupling of vibrations to the thermal bath. The other nonequilibrium effect which should be taken into account is spectrum modification due to nonequilibrium distribution function of electrons at finite voltage.

Pause

TT 33.8 Di 16:00 TU H3027

Theoretical analysis of conductance histograms of Au atomic contacts — •F. Pauly[1], M. Dreher[2], J.C. Cuevas[1], E. Scheer[2], and P. Nielaba[2] — [1]Institut für Theoretische Festkörperphysik, University of Karlsruhe, 76128 Karlsruhe, Germany — [2]Physics Department, University of Konstanz, 78457 Konstanz, Germany

Many experiments have shown that the conductance histograms of metallic atomic-sized contacts exhibit a peak structure, which is characteristic of the corresponding material. In order to shed some light on the origin of these peaks, we present a theoretical analysis of the conductance histograms of Au atomic contacts, investigating the interplay between mechanical and electrical properties of these nanocontacts. We have combined classical molecular dynamics simulations of the breaking of nanocontacts with conductance calculations based on a tight-binding model. This combination gives us access to crucial information such as contact geometries, forces, minimum cross section, total conductance and transmission coefficients of the individual conduction channels. We also compare with experimental results on Au atomic contacts where the individual channel transmissions have been determined.

TT 33.9 Di 16:15 TU H3027

Utilization of Carbon Nanotubes by Surface Acoustic Waves — •Jens Ebbecke[1], Christoph J. Strobl[2], and Achim Wixforth[1] — [1]Institut für Physik der Universität Augsburg, Experimentalphysik I, Universitätsstr. 1, 86135 Augsburg — [2]Sektion Physik der Ludwig-Maximilian-Universität und Center for Nanoscience (CeNS), Geschwister-Scholl-Platz 1, 80539 München

We report a surface acoustic wave (SAW) mediated carbon nanotube (CNT) alignment parallel to the sample surface. The piezoelectric field of the SAW aligns the CNTs in parallel to the wave vector. Furthermore we have contacted single-walled CNTs after aligning them. The acoustoelectric current has been measured at 4.2 K and a probing of the low-dimensional electronic states by the SAW has been detected. By decreasing the acoustic wavelength resulting in an adjustment to the length of the defined CNT constriction a quantization of the acoustoelectric current has been observed.

TT 33.10 Di 16:30 TU H3027

Magnetoconductance in Disordered Carbon-Nanotubes — •Norbert Nemec and G. Cuniberti — Molecular Computing Group, Universität Regensburg, Germany

Single wall carbon-nanotubes in tight-binding approximation are one of the simplest nontrivial theoretical models with physical relevance that can be used for studying quantum mechanical transport mechanisms at the molecular scale. Based on this this model, we examine the interplay of disorder with external magnetic fields, leading to signs of weak localization. As expected, weak localization is enhanced in the energy regions with high density of states. We quantify the resulting energy dependent mean free path in relation to the sample size and the strength of the disorder. "Coating wideband leads" are introduced as a novel approach to model realistic contacts as they are found in experiment, without adding much computational complexity.

TT 33.11 Di 16:45 TU H3027

Non-linear transport properties in commensurate and incommensurate double-walled carbon nanotubes — •Shidong Wang and Milena Grifoni — Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

We use a tight-binding model to investigate the effective intershell coupling in double-walled carbon nanotubes. We derive an analytical expression for the effective intershell coupling and find selection rules. The intershell coupling between lowest bands is significantly suppressed if two shells are incommensurate. Including the long-ranged Coulomb interactions, double-walled carbon nanotubes can be described by Luttinger liquid theory at low energies. The tunneling density of states and the non-linear I-V characteristics of double-walled carbon nanotubes are also obtained.

TT 33.12 Di 17:00 TU H3027

Franck-Condon blockade and giant Fano factors in transport through single molecules — •Jens Koch and Felix von Oppen — Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

We show that Franck-Condon physics leads to a significant current suppression at low bias voltages (termed Franck-Condon blockade) in transport through single molecules with strong coupling between electronic and vibrational degrees of freedom.

For weak vibrational relaxation, we find that transport in this regime is characterized by remarkably large Fano factors (10^2–10^3), which arise due to avalanche-like transport of electrons. Avalanches occur in a self-similar manner over a wide range of time scales, as reflected in power-law dependences of the current noise on frequency and vibrational relaxation rate.

TT 33.13 Di 17:15 TU H3027

Transport calculations for single molecules based on density functional theory: some fundamentals — •F. Evers[1], K. Burke[2], and R. Gaudoin[2] — [1]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany — [2]Department of Chemistry and Chemical Biology, Rutgers University, 610 Taylor Road, Piscataway NJ 08854

In principle, the use of time dependent density functional theory (TDDFT) allows for exact calculations of the linear and non-linear density and current response of interacting many-body systems. An important application of this method are transport calculations for single molecules. In practice, one is forced to make approximations for the exchange correlation (XC) functional employed which then can put serious limits to the accuracy of TDDFT calculations. We will discuss artifacts that can occur if the non-equilibrium XC-functional is replaced by the equilibrium one. A formalism will be proposed that allows to include the XC-functional in the hydrodynamic approximation (Vignale and Kohn) into the standard DFT-approach to transport.

TT 33.14 Di 17:30 TU H3027

Electron and Exciton Transfer in Donor-Acceptor Systems: Many-Particle Effects and Influence of Electronic Correlations — •Sabine Tornow, Ning-Hua Tong, and Ralf Bulla — Theoretische Physik III, Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

The spin boson model provides a well established description of electron transfer processes from a donor to an acceptor. The redox sites are modelled by two localized quantum states. This picture breaks down in multi electron transfer processes if many particle effects and electron correlations have to be taken into account. We present a theoretical non-perturbative study of the electron and exciton transfer based on an extended spin boson model where the redox sites are modelled more realistically. Using Wilsons Numerical Renormalization Group method we discuss effects of the electron correlations on the transfer rate.