Influence of disorder and dephasing events on the electron transport through conjugated molecular wires in molecular junctions — Claudia Gomes da Rocha, Ho-racio M. Pastawski, and Gianaurelio Cuniberti

Master-equation approach for simulating STM images of single molecules — Jens Kortus

Molecular orbital switching in photochromic single molecular junctions — Youngsang Kim, Torsten Pietzsch, Elke Scheren, Thomas Helli-muth, Fabian Pauly, Dmitro Sysoiev, Thomas Huhn, Thomas Ender, Ulrich Grotth, Ulrich Strüken, and Artur Ermin

Molecular orbital switching in photochromic single molecular junctions — Youngsang Kim, Torsten Pietzsch, Elke Scheren, Thomas Helli-muth, Fabian Pauly, Dmitro Sysoiev, Thomas Huhn, Thomas Ender, Ulrich Grotth, Ulrich Strüken, and Artur Ermin

Spin-polarized transport through single-molecule junctions: insight from theory — Alexei Bagrets and Ferdinand Evers

Vibrationally dependent electron-electron interactions in single-molecule junctions: A mechanism for asymmetric gate-voltage dependence of the current in symmetrically coupled junctions — Kainer Hütte, Andre Erpenbeck, and Michael Thoss

Transport through \( \pi \)-stacked benzene rings and evaluation of their IETS — Thomas Hellmuth, Marcus Büttke, Fabian Pauly, and Gerd Schön

Photoswitchable molecules gain significant interest due to the applicability in data storage media, as optical switches, and in novel logic circuits [1]. The molecular energy levels and their coupling to the metal leads on both the single-molecule conductance and the switching ratio between the two states of a switch molecule. Here, we show the preferential conductance of individual, specifically designed sulfur-free diarylithene molecules in photodetectors and the switching ratio between the two states of a switch molecule. Here, we discuss the changes in the differential conductance (I-V) characteristics using the single-level model [3].


In this talk, a short overview will be given on our recent advances in DFT modeling of spin-polarized electron transport across single molecules bridged between magnetic reservoirs. In particular, we will discuss implementation of the non-equilibrium Green’s function for-
malism, where efficient absorbing boundary conditions encoded into self-energy function are extended to account for the spin-polarized electronic structure of magnetic electrodes. We will demonstrate an ability, within our approach, to treat a variety of different magnetic configurations (e.g. nano-scale domain walls) which could appear when a molecule with few spin-centers (d-ions) is brought in contact with a magnetic surface and a tip of the spin-polarized-STM. Recent experiments [1,2] on spin-transport and magnetoresistance effect observed in hydrogen-phtalocyanine STM molecular junctions will be discussed in detail.


TT 32.8 Wed 17:00 BH 334

Optical response of a single-molecule junction: current switching, negative differential resistance and plasmon-induced conductance enhancement — •YAROSLAV ZELINSKY1,2 and VOLKARD MAY1 — 1Institut für Physik, Humboldt Universität zu Berlin, Newtonstrasse 15, D-12489 Berlin, Germany — 2Bogolubov Institute for theoretical physics National Academy of Science of Ukraine. Metrologichna str. 14b, UA-03683, Kiev, Ukraine

Based on a generalized master equation approach the conductive properties of a current-carrying molecular junction driven by an external optical excitation are studied [1]. The description incorporates vibrational states of the molecule and related relaxation processes with the latter being crucial for the strength of the actual current. A photoinduced switch of the current, the appearance of a negative differential resistance and its photoinduced suppression are predicted [2]. The nano-electrode plasmon control of the single molecule conductivity appearing at the simultaneous optical excitation of the molecule and the electrodes is also considered [3]. A remarkable enhancement of the current is achieved in this case.


TT 32.9 Wed 17:15 BH 334

Resonant photoconductance of molecular junctions formed in Gold nano-particle arrays — M. MANGOLD1, J. SCHOPKA1, M. CALAME2, M. MAYOR3, and A.W. HOLLEITNER1 — 1Walter Schottky Institut and Physik-Department, Technische Universität München, 85748 Garching — 2Departement Physik, Universität Basel, 4056 Basel, Switzerland — 3Department Chemie, Universität Basel, 4056 Basel, Switzerland

We report on a molecular phototransistor effect based on oligo(phenylene vinylene) (OPV) incorporated in gold nanoparticle arrays. We find a pronounced photoconductance arising upon resonant excitation of the OPV molecules. We determine the typical response time and the irradiation intensity dependence of this resonant photoconductance. Our results suggest that the charge carriers, which are resonantly excited in the OPV molecules, directly contribute to the current flow through the nanoparticle arrays. We can consistently model the dynamics of the resonant photoconductance by considering the filling and recombination of trap states in the nanoparticle arrays. Our results verify that individual molecules in metal-molecule-metal junctions can be functional modules of optoelectronic devices [1].