

**tact** — •VELIMIR MEDED, ALEXEJ BAGRETS, ANDREAS ARNOLD, and FERDINAND EVERS — Institute of Nanotechnology, Research Centre Karlsruhe, Hermann-von-Helmholtzplatz 1, 76344 Eggenstein-Leopoldshafen, Germany

Two experiments measuring the current-voltage characteristics (IV) of the bipyridine-dinitro-dithiole-system found that the molecule can be controllably switched between two states exhibiting significantly different IV curves [1,2]. To better understand the nature of the bistable state we have performed ab initio calculations. They indicate, that molecular charging/uncharging does not lead to bistability in the presence of electrodes. By contrast, two (or more) energy minima can arise with conformational changes of the molecule alone or in the molecule-contact region (possibly combined with structural relaxations in a larger contact area). As a prototypical example of such a mechanism, we consider rotations of the molecule about the axis defined by the two anchoring Au-atoms. From an extensive analysis of possible contact structures, we conclude that bistable configurations can indeed arise for slightly disordered, i.e. realistic, contacts – though they do not appear to be generic. A scenario will be proposed, how in this light experimental findings might be understood. (We are indebted to E. Loertscher, H. Riel and M. Ruben for instructive discussions.)

[1] Z. K. Keane, J. W. Ciszek, J. M. Tour, and D. Natelson, *Nano Lett.*, Vol. 6, No. 7, 2006. [2] E. Lörtscher, J. W. Ciszek, J. Tour, and H. Riel, *Small* 2, 973 (2006).

TT 14.9 Tue 11:45 H 3010

**Temperature dependence of the conductance in biphenyl-dithiol single-molecule junctions** — •FABIAN PAULY<sup>1</sup>, JANNE VILJAS<sup>1,2</sup>, JUAN CARLOS CUEVAS<sup>3</sup>, and GERD SCHÖN<sup>1,2</sup> — <sup>1</sup>Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures, Universität Karlsruhe, 76128 Karlsruhe, Germany — <sup>2</sup>Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe, Germany — <sup>3</sup>Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, 28049 Madrid, Spain

Using a density-functional-based transport method, we study the conduction properties of several biphenyl-derived dithiol (BPDDT) molecules wired to gold electrodes [1]. The BPDDT molecules differ in their side groups, which control the degree of conjugation of the  $\pi$ -electron system. We have analyzed the dependence of the low-bias zero-temperature conductance on the tilt angle  $\varphi$  between the two phenyl ring units, and find that it follows closely a  $\cos^2(\varphi)$  law as observed in a recent experiment [2].

In addition, we study the temperature dependence of both the conductance and its fluctuations and find qualitative differences between the examined molecules. We illustrate that the fluctuations of the conductance due to temperature-induced changes in the geometric structure of the molecule can be reduced by an appropriate design.

[1] F. Pauly, J. K. Viljas, J. C. Cuevas, G. Schön, arXiv:0705.3285.

[2] Venkataraman *et al.*, *Nature* 442, 904 (2006).

TT 14.10 Tue 12:00 H 3010

**Symmetry effects in transport properties of benzene quantum dots** — •GEORG BEGEMANN, DANA DARAU, ANDREA DONARINI, and MILENA GRIFONI — Theoretische Physik, Universität Regensburg

We investigate electronic transport through a benzene molecule quantum dot. In particular, we investigate the influence of the contacts' position and find qualitative and quantitative differences between the para- and the meta configurations.

The Hamiltonian of the interacting isolated molecule is diagonalized and its eigenstates are classified according to their particle number, spin and symmetry representation.

Treating the coupling to the leads perturbatively, a generalized master equation for the reduced density matrix in the benzene's eigenbasis is derived, which includes coherences between degenerate eigenstates. We explicitly demonstrate that the coherences do not contribute to the linear transport, but become essential for the meta-configuration in the nonlinear regime.

Analytic expressions for the linear conductance and the current in

the low bias regime agree with numeric calculations, where we are not restricted to small voltages. Interesting features appear over a wide range of gate and bias voltages, for example, due to the reduced symmetry of the problem, negative differential conductance is present in the meta-configuration, while it is absent in the para-configuration.

TT 14.11 Tue 12:15 H 3010

**Vibrational Effects in Electron Transport through Molecular Junctions** — •RAINER HÄRTLE, CLAUDIA BENESCH, and MICHAEL THOSS — Institut für Theoretische Chemie, Technische Universität München, D-85747 Garching, Germany

We investigate theoretically the role of vibrations in electron transport through single molecule junctions. The study is based on a generic model, which describes steady-state transport through a single molecule that is attached to metal leads. To address multidimensional vibrational dynamics in molecular junctions, we have extended the non-equilibrium Green function approach established by M. Galperin *et al.* to multiple modes. We demonstrate the effect of electronically induced coupling between different vibrational modes and study the stability of these junctions by calculating the vibrational excitations as a function of the bias voltage. In addition to a model system with two vibrational degrees of freedom, we present results for *p*-benzenedi(butanethiolate) covalently bound to gold electrodes.

TT 14.12 Tue 12:30 H 3010

**Quantum fluctuations and vibration-assisted transport through single molecule transistors** — •MARTIN LEIJNSE<sup>1,2</sup>, MAARTEN WEGEWIJS<sup>1,2</sup>, and HERBERT SCHOELLER<sup>1</sup> — <sup>1</sup>Institut für Theoretische Physik A, RWTH Aachen, 52056 Aachen, Germany — <sup>2</sup>Institut für Festkörper-Forschung - Theorie 3, Forschungszentrum Jülich, 52425 Jülich, Germany

Non-equilibrium transport through a single molecule transistor is studied in the presence of strong coupling to a local vibrational mode. Employing a full fourth order perturbation expansion in the tunneling Hamiltonian, we address the experimentally relevant regime of intermediate tunneling coupling between molecule and electrodes. Using the real-time transport theory we calculate the nonlinear conductance, accounting for the so-called cotunneling contributions, as well as renormalization and broadening effects, induced by charge fluctuations. We find that broadening and in-elastic cotunneling processes are of comparable importance for the lifting of the vibration-induced Franck-Condon blockade. Strikingly, novel transport features connected to this broadening are found below the bias-voltage threshold for in-elastic cotunneling, which have gone unnoticed until now. Relaxation of the vibrational distribution, induced by coupling to an external phonon bath, leads to a uniform reduction of all higher order processes, i.e. broadening and in-elastic effects remain comparable.

TT 14.13 Tue 12:45 H 3010

**Charge-memory effect in molecular junctions** — •PINO D'AMICO<sup>1</sup>, DMITRY A. RYNDYK<sup>1</sup>, GIANAURELIO CUNIBERTI<sup>2</sup>, and KLAUS RICHTER<sup>1</sup> — <sup>1</sup>Institut für Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany — <sup>2</sup>Max Bergmann Centre for Biomaterials, Dresden University of Technology, D-01062 Dresden, Germany

Charge-memory effects such as bistability and switching between a charged and a neutral state, have been recently observed in an increasing number of experiments on charge transport through molecules [1,2]. We consider a charge-memory effect in the framework of a minimal polaron model. It is shown that in the case of strong electron-vibron interaction the rate of spontaneous quantum switching between two metastable states is exponentially suppressed at zero bias voltage, while remaining large enough at finite voltage. The switching between states at finite voltage and hysteretic charge-voltage curves are calculated at weak coupling to the leads by the master equation method, and at stronger coupling to the leads by the equation-of-motion method for nonequilibrium Green functions.

[1] Jascha Repp *et al.*, *Science*, vol 35, 493-495 (2004)

[2] F. E. Olsson *et al.*, *PRL*, vol 98, 176803 (2007)