

**MA 43: Transport: Molecular Electronics and Photonics 2**  
**(Joint session of CPP, DS, HL, MA, O and TT organized by TT)**

Time: Thursday 15:00–16:00

Location: H23

MA 43.1 Thu 15:00 H23

**First-principles calculation of the thermoelectric figure of merit for [2,2]paracyclophane-based single-molecule junctions** — •MARIUS BUERKLE<sup>1</sup>, FABIAN PAULY<sup>2</sup>, and YOSHIHIRO ASAI<sup>1</sup> — <sup>1</sup>AIST Tsukuba — <sup>2</sup>University Konstanz

Here we present a theoretical study of the thermoelectric transport through [2,2]paracyclophane-based single-molecule junctions [1]. Combining electronic and vibrational structures, obtained from density functional theory (DFT), with nonequilibrium Green's function techniques allows us to treat both electronic and phononic transport properties at a first-principles level. Paracyclophane derivatives offer a great flexibility in tuning their chemical properties by attaching different functional groups. We show that, for the specific molecule, the functional groups mainly influence the thermopower, allowing us to tune its sign and absolute value. We predict that the functionalization of the bare paracyclophane leads to a largely enhanced electronic contribution Z<sub>e</sub>T to the figure of merit. Nevertheless, the high phononic contribution to the thermal conductance strongly suppresses ZT. Our work demonstrates the importance to include the phonon thermal conductance for any realistic estimate of the ZT for off-resonant molecular transport junctions.

[1] M. Buerkle et al., PRB **91**, 165419 (2015)

MA 43.2 Thu 15:15 H23

**Switching the conductance of a molecular junction by proton transfer** — •DOMINIK WECKBECKER, PEDRO B. COTO, CHRISZANDRO HOFMEISTER, and MICHAEL THOSS — Institut für Theoretische Physik, Staudtstraße 7/B2, 91058 Erlangen, Germany

The idea of designing switches or diodes using single molecules has motivated intensive experimental and theoretical research on the conductance properties of these systems. In particular, it has been demonstrated that a molecular junction may be used as a nanoswitch if the molecular bridge has two stable states with different conductance that can be reversibly transformed into each other [1]. In this contribution, we explore the possibility of switching a molecular junction using a proton transfer reaction triggered by an external electrostatic field [2]. The study uses transport theory based on first-principles electronic structure calculations [2,3] and considers molecular junctions with graphene or gold as material for electrodes. We show that for the systems investigated, proton transfer can be used for the reversible interconversion between two states, which exhibit different degrees of delocalization of the  $\pi$ -electrons and therefore very different conductance.

[1] S. J. van der Molen et al., J. Phys.: Cond. Mat. **22**, 133001 (2010)[2] C. Hofmeister et al., J. Mol. Model. **20**, 2163 (2014)[3] M. Brandbyge et al., PRB **65**, 165401 (2002)

MA 43.3 Thu 15:30 H23

**Design rules for molecular electronics: Diarylethene**

**molecules und derivatives** — •LOKAMANI LOKAMANI<sup>1</sup>, TORSTEN SENDLER<sup>1</sup>, PETER ZAHN<sup>1</sup>, SIBYLLE GEMMING<sup>1,2</sup>, and ARTUR ERBE<sup>1</sup> — <sup>1</sup>Helmholtz-Zentrum Dresden-Rossendorf e.V., 01314 Dresden, Germany. — <sup>2</sup>Institute of Physics, Technische Universität, 09107 Chemnitz, Germany.

Diarylethenes, a class of photosensitive molecules which exhibit photochromism, can be switched between open- and closed-ring isomers. In break-junction experiments diarylethene derivatives [1] in open and closed-ring forms can be distinguished by a low and high conductance state respectively with a difference in current levels of about one order of magnitude. In addition, these molecules exhibit stable electrical characteristics in both conductance states. Here, we study the electronic transport properties of such derivatives at the level of single molecules. In particular, we analyze the effect of various electron accepting and donating groups on the conductance properties of single molecules attached to gold electrodes. We explore the underlying design rules for molecular electronics comparing break-junction experiments and the theoretical investigations on diarylethene molecules and derivatives.

[1] T. Sandler et al., Advanced Science **2**, 1500017 (2015)

MA 43.4 Thu 15:45 H23

**Experimental investigation of the role of electron-phonon-coupling on the Mott critical behavior in the organic charge-transfer salts  $\kappa$ -(BEDT-TTF)<sub>2</sub>X** — •E. GATI<sup>1</sup>, M. GARST<sup>2</sup>, R.S. MANNA<sup>1</sup>, U. TUTSCH<sup>1</sup>, B. WOLF<sup>1</sup>, S. HARTMANN<sup>1</sup>, L. BARTOSCH<sup>3</sup>, T. SASAKI<sup>4</sup>, H. SCHUBERT<sup>1</sup>, J.A. SCHLUETER<sup>5</sup>, and M. LANG<sup>1</sup> — <sup>1</sup>Physikalisches Inst., Goethe Uni, SFB/TR49, Frankfurt, DE — <sup>2</sup>Inst. f. Theo. Physik, Universität zu Köln, DE — <sup>3</sup>Inst. f. Theo. Physik, Goethe Uni, FfM, DE — <sup>4</sup>IMR, Tohoku University, Sendai, Japan — <sup>5</sup>Materials Science Division, Argonne National Laboratory, USA

The Mott transition is one of the key phenomena of strongly correlated electron systems. Of fundamental interest is the determination of its critical behavior and the underlying universality class. Despite intensive experimental efforts, the universality class is still unresolved. A key aspect, which has not been addressed in these approaches, is the role of electron-phonon-coupling as it is supposed to alter the critical properties to Landau criticality [1]. We will present thermal expansion studies under pressure [2] on the organic charge-transfer salt  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu[N(CN)<sub>2</sub>]Cl. This technique is a very sensitive tool to detect critical behavior [3] as well as influences of the lattice on the electronic subsystem [1]. Our results clearly show a breakdown of Hooke's law of elasticity which is a direct evidence for significant electron-phonon-coupling. Furthermore, we will discuss its effect on the critical exponents determined by this thermodynamic probe.

[1] Zacharias et al., PRL **109**, 176401 (12)[2] Manna et al., Rev. Sci. Instrum. **83**, 085111 (2012)[3] de Souza et al., PRL **99**, 0370031 (2007)