

## TT 72: Transport: Molecular Electronics II

Time: Wednesday 15:00–16:15

Location: HSZ 304

TT 72.1 Wed 15:00 HSZ 304

**Conductance and thermopower of long molecular wires** — ●F. ROCHAU<sup>1</sup>, M. KOTIUGA<sup>2,3</sup>, T. J. HELLMUTH<sup>4</sup>, J. B. NEATON<sup>2,3</sup>, and F. PAULY<sup>1</sup> — <sup>1</sup>Department of Physics, University of Konstanz, Germany — <sup>2</sup>Molecular Foundry, Lawrence Berkeley National Laboratory, California, USA — <sup>3</sup>Department of Physics, University of California, Berkeley, USA — <sup>4</sup>Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, Germany

We study the transition from coherent tunneling to incoherent hopping for the conductance  $G$  and the thermopower  $S$  of long molecular wires [1]. Using a tight-binding model for the electronic structure combined with Green's function techniques to describe transport, we include dephasing by means of Büttiker probes. We discuss the one-dimensional chain as well as several benzene-based molecular junctions (oligophenylenes, polyacenes and polyphenanthrenes). For the one-dimensional chain we derive analytical formulas for the length dependence of the phase-coherent  $G$  and  $S$ , distinguishing off-resonant, band-edge, and on-resonant transport. Irrespective of the regime and the system considered, we find an ohmic inverse length dependence of  $G$  and a saturating  $S$  for long molecular wires, when dephasing is included. The power factor  $S^2G$  of long wires is therefore determined by  $G$ . Finally, we study the huge thermopower resulting from transmission nodes for the polyphenanthrenes and observe how they disappear when decoherence is added.

[1] F. Rochau, M. Kotiuga, T. Hellmuth, J. B. Neaton, and F. Pauly, in preparation

TT 72.2 Wed 15:15 HSZ 304

**Noncollinear electronic transport through star-shaped Fe<sub>4</sub> nanomagnet** — ●VOLODYMYR V. MASLYUK<sup>1</sup>, LEONID SANDRATSKII<sup>2</sup>, and INGRID MERTIG<sup>1,2</sup> — <sup>1</sup>Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — <sup>2</sup>Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

During the last decade single molecular magnets have attracted huge interest because of their spectacular magnetic properties. Here we present a theoretical investigation of the star-shaped Fe<sub>4</sub>(OMe)<sub>6</sub>(dpm)<sub>6</sub> nanomagnets placed between ferromagnetic Co(100) electrodes. We use the combination of the NEGF method and the density-functional theory realized in the TranSIESTA code [1] and adapted for the investigation of the magnetic systems with non-collinear magnetic order. We take into account electron-correlations effects via a Hubbard-like term that was added to our DFT functional. We found that the Fe<sub>4</sub> molecule has a magnetic moment of 10  $\mu_B$  in the ground state. We also obtain that the magnetic anisotropy barrier of the molecule is small, 0.33 meV, that allows us to neglect the spin-orbit interaction in the transport properties calculations. The molecule placed between electrodes tends to be antiferromagnetically aligned with the magnetization of the leads. We show that the direction of the magnetization of the molecule changes with the variation of the relative directions of the magnetization of the leads. This has an impact on the transmission spectra of the system.

[1] M. Brandbyge, *et al*, Phys. Rev. B 65, 165401 (2002)

TT 72.3 Wed 15:30 HSZ 304

**Localization under the effect of randomly distributed decoherence** — ●THOMAS STEGMANN<sup>1</sup>, ORSOLYA UJSÁGHY<sup>2</sup>, and DIETRICH E. WOLF<sup>1</sup> — <sup>1</sup>Department of Physics and CENIDE, University of Duisburg-Essen, Germany — <sup>2</sup>Department of Theoretical Physics, Budapest University of Technology and Economics, Hungary

Electron transport through disordered quasi one-dimensional quantum systems is studied. Decoherence is taken into account by a spatial distribution of virtual reservoirs, which represent local interactions of the conduction electrons with their environment.

We show that the decoherence distribution has observable effects on

the transport. If the decoherence reservoirs are distributed randomly without spatial correlations, a minimal degree of decoherence is necessary to obtain Ohmic conduction. Below this threshold the system is localized and thus, a decoherence driven metal-insulator transition is found. In contrast, for homogeneously distributed decoherence, any finite degree of decoherence is sufficient to destroy localization. Thus, the presence or absence of localization in a disordered one-dimensional system may give important insight about how the electron phase is randomized.

[1] arXiv:1308.4328

TT 72.4 Wed 15:45 HSZ 304

**Electronic and Structural Properties of Functionalized Nanoparticle Networks: A Multi-Scale Approach** — ●TAHEREH GHANE<sup>1</sup>, DAIJIRO NOZAKI<sup>1</sup>, AREZOO DIANAT<sup>1</sup>, RAFAEL GUTIERREZ<sup>1</sup>, and GIANAURELIO CUNIBERTI<sup>1,2,3</sup> — <sup>1</sup>Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany — <sup>2</sup>Center of Advancing Electronics Dresden, TU Dresden, Germany — <sup>3</sup>Dresden Center for Computational Materials Science, TU Dresden, Germany

Functionalized nanoparticle networks offer a model system for the study of charge transport in low-dimensional systems as well as a potential platform to implement electronic functionalities. The electrical response of a nanoparticle network is expected to sensitively depend on the molecular inter-connects, i.e. on the linker chemistry. If these linkers have complex charge transport properties as is the case of molecular switches with conformational dependent electronic properties or molecular memristors showing hysteretic behavior, then phenomenological models addressing the large scale properties of the network need to be complemented with microscopic calculations of the network building blocks. In this study we investigate the electronic, structural and charge transport properties of functionalized nanoparticle by employing a multi-scale method in which we combine density-functional based approaches, classical molecular dynamics, and charge transport calculations.

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TT 72.5 Wed 16:00 HSZ 304

**Influence of structural distortions on the polarization function in molecular-based quantum cellular automata: a minimal model approach** — ●ALEJANDRO SANTANA<sup>1,2</sup>, RAFAEL GUTIERREZ<sup>1,2</sup>, and GIANAURELIO CUNIBERTI<sup>1,2</sup> — <sup>1</sup>Institute for Materials Science and Max Bergmann Center of Biomaterials, 01062 Dresden, Germany. — <sup>2</sup>Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany.

Molecular Quantum Cellular Automata (m-QCA) offers a new paradigm in which information can be encoded using special geometrical arrangements of charges within one of the m-QCA cell and transmitted by cell-cell interaction between nearest neighbors. In fact, m-QCA implementation relies on three basic assumptions (a) charge localization within the molecule, (b) switching between two possible electronic states and (c) electrostatic coupling between nearest-neighbors. Therefore, under those conditions, functionality of m-QCA implies a complex relationship between quantum mechanical effects, such as electron transfer (ET) processes within the molecule, and electrostatic interactions between cells. Fundamental questions about the impact of structural distortions of individual m-QCA are addressed and allowing us to formulate a response function in which the geometry of the system and the ET coupling are used as effective parameters. Our study indicates that even small changes in the original geometry of the system have a dramatic impact on the cell response and, therefore, changing the idea of the QCA-network implementation when is compared with the classical paradigm.