TT 51: Molecular Electronics and Photonics (joint session TT/CPP)

Time: Wednesday 18:00–19:00 Location: HSZ 304

TT 51.1 Wed 18:00 HSZ 304

Efficient steady state solver for charge transport through single-molecule junctions — •Christoph Kaspar and Michael Thoss — Albert-Ludwigs-Universität, Freiburg, Germany

The steady state is a fundamental property used to describe the non-equilibrium transport of electrons through single-molecule devices. Its rigorous computation requires highly accurate methods such as the hierarchical quantum master equation approach [1,2]. This method gives access to the systematic inclusion of higher-order contributions resulting in the generalization of perturbative master equation approaches. The major disadvantage of calculating the steady state with this method is the excessive requirement of computational resources, e.g. needed for increasing strength of molecule-lead coupling or many molecular degrees of freedom [3,4]. In this contribution, we present an iterative approach enabling the efficient computation of the steady state for the transport through single-molecule junctions. Besides reducing the required computational time, the main benefit is a drastically decreased memory compared to conventional propagation schemes. We demonstrate the efficiency of our iterative approach on the scenario of a single-molecule junction with many system degrees of freedom.

[1] Jin *et al.*, J. Chem. Phys. **128**, 234703 (2008)
[2] Schinabeck *et al.*, Phys. Rev. B **94**, 201407R (2016)
[3] Hou *et al.*, J. Chem. Phys. **142**, 104112 (2015)
[4] Zhang *et al.*, J. Chem. Phys. **147**, 044105 (2017)

TT 51.2 Wed 18:15 HSZ 304

Low temperature single molecule transport measurements on fullerenes — •Alexander Strobel[1,2], Filip Kilibarda[1,2], Elke Scheer[2], and Artur Erbe[1,2] — [1]Helmhotz Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]University of Konstanz, Faculty of sciences, 78457 Konstanz, Germany

Molecular electronics offers a novel approach, for scaling traditional 3D electronics down to nanoscale dimensions in a quasi 1D system. This approach offers a deeper understanding of the electron transport behavior of molecules. Our research focuses on classifying different molecules with the help of Mechanically Controlled Break Junction (MCBJ) technique. Here we report electrical transport properties of fullerene molecules using a MCBJ setup. Fullerenes with their high stability and symmetry have become reference molecules for the development of measurement routines for molecular electronics applications. Our MCBJ setup enables us to evaporate C60 in situ and measure electrical characteristics under high vacuum conditions. Furthermore, low-temperature measurements down to 6 K are possible. Conductance histograms are recorded to measure the preferred conductance values of single C60 molecules. I-V curves, the differential conductance and inelastic electron tunneling spectra (IETS) are directly and simultaneously measured using lock-in measurement methods. IETS measurements are used to investigate electron-phonon Interactions. The experimental analysis of the charge transport by varying the electrode distance, the bias potential and the electrode metal at different conductance is presented.

TT 51.3 Wed 18:30 HSZ 304

Ab initio study of current-induced forces in nanojunctions — •Susanne Leitherer[1], Nick Papior[2], Jing-Tao Lü[3], and Mads Brandbyge[1] — [1]Department of Physics, Technical University of Denmark — [2]Department of Applied Mathematics and Computer Science, Technical University of Denmark — [3]School of Physics, Huazhong University of Science and Technology, Wuhan, China

In ballistic nanoscale conductors the high current density can lead to substantial changes in the atomic structure, as seen in experiments [1]. We calculate the current-induced forces on the atoms of different models of nanojunctions under a high applied bias voltage, employing first principles electronic structure and transport calculations. Our findings show how the forces on the atoms are related to the chemical bonds, as evidenced in scanning probe experiments exploring currents and forces between two C_{60} molecules [2], as well as the electrostatic potential landscape in the junctions [3]. To study further the dynamical motion of atoms in nanojunctions including current-induced forces, we perform molecular dynamics simulations based on a semi-classical Langevin approach in combination with DFT calculations [4]. This allows us to study the influence of Joule heating, i.e. inelastic scattering by phonons, as well as other contributions to current-induced forces that do not conserve the energy of the atomic motion.

[1] C. Schirm et al., Nat. Nanotechnol. 8, 645-648 (2013)
[2] J. Brand et al., Nano Lett. 19, 7845-7851 (2019)
[3] S. Leitherer et al.,Phys. Rev. B 100, 035415 (2019)
[4] J.T. Lü et al., Manuscript in preparation

TT 51.4 Wed 18:45 HSZ 304

Electrical transport through single polypeptides — •Diana Slawig[1], Nguyen Thi Ngoc Ha[2], Yossi Paltiel[3], Shira Yoshelis[3], and Christoph Tegenkamp[1,2] — [1]Leibniz Universität Hannover, Germany — [2]TU Chemnitz, Germany — [3]Hebrew University Jerusalem, Israel

The analysis of electrical transport through helical molecules gained a lot of interest within the last years, due to the unique spin filtering properties, named chiral induced spin selectivity (CISS) [1]. By utilizing this effect a proof of concept for a new type of chiral-based Si-compatible universal magnetic memory device was demonstrated [2]. Nevertheless, the electrical transport through helical peptides itself is not completely understood yet.

Our study focuses on transport through single lysine doped polyalanine (PA) molecules by means of mechanically controlled break junction. Molecular fragments containing different numbers of monomers were used to evaluate the length dependent transport behavior, leading to a strong indication for a tunneling dominated mechanism.

Based on the high number of observed stable conductance states in the statistical analysis, we propose a ratcheting model based on geometrical alignments of the molecules. This concept is closely related to the interdigitation effect observed by STM[3].

[1] R. Naaman et al., J. Phys. Chem. Lett., 3 (2012)
[2] O.Ben Dor et al., Nat. Commun. 4:2256 (2013)
[3] T. N.H. Nguyen et al., J. Phys. Chem. C 123, 612 (2019)