

TT 16: TR: Nanoelectronics III - Molecular Electronics 1

Time: Monday 18:15–19:45

Location: HSZ 03

TT 16.1 Mon 18:15 HSZ 03

Thermal conductivity behavior in double-stranded molecular systems — ●ELENA DIAZ, RAFAEL GUTIERREZ, and GIANAURELIO CUNIBERTI — Institute for Materials Science, Dresden University of Technology, 01062 Dresden, Germany

The analysis of the mechanisms mediating energy flow in biomolecules is a fundamental issue for the understanding of many biologically relevant functions. Our interests focus on studying the energy and heat transport along biomolecular systems which present helix structures, i. e. alpha-helices in proteins or double-helix DNA. When dealing with such systems, the anomalous thermal properties of low dimensional systems must be taken into account. For instance, it is well known that one dimensional harmonic lattices are not able to present the proper thermal gradient in a non-equilibrium regime. Furthermore, even when anharmonicity is present in the system, Fourier's law is still not valid unless a local potential affects every site of the lattice. Biomolecular systems, specially those containing helix structures, can be considered as ladder models of coupled one-dimensional lattices. In this work we study how the thermal properties of isolated lattices are modified by introducing this coupling. We demonstrate that a harmonic lattice interacting with an anharmonic system is able to support a well defined thermal gradient for a large enough coupling. Our results show that by coupling two lattices with a different strength of anharmonicity heat rectification features can arise.

TT 16.2 Mon 18:30 HSZ 03

Electronic signatures of DNA with oxidative damage(8-oxoguanine) — ●MYEONG LEE¹, GIORGIA BRANCOLINI², RAFAEL GUTIERREZ¹, and GIANAURELIO CUNIBERTI¹ — ¹Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062, Dresden, Germany — ²National Research Center on nanoStructures and bioSystems at Surfaces (S3) of INFN-CNR, Via Campi 213/A, 41100 Modena, Italy

8-Oxoguanine (8-oxoG) is the most common form of oxidative DNA damage found in human cells. When DNA polymerases encounter 8-oxoG, they frequently misincorporate adenine in preference to cytosine, leading to G:C → T:A transversion mutation which is commonly found in age-related diseases and human cancers. How DNA repair enzymes recognize 8-oxoG lesions within the entire genome is a long-standing question. Recent experiment by Markus *et al.* [1] suggests that electronic property of 8-oxoG might play a role in the mechanism of locating damage. In this talk we discuss the electronic structure and charge transfer characteristics of dsDNA sequence with 8-oxoG:C and 8-oxoG:A base pairs compared to the one with regular base pairs (G:C). We fully consider the effect of solvent environment and structural fluctuations [2] by combining molecular dynamics (MD) simulations and electronic structure calculations.

[1] T.Z. Markus *et al.*, J. Am. Chem. Soc. **131**, 89 (2008).

[2] P. B. Woiczikowski *et al.*, J. Chem. Phys. **130**, 215104 (2009); R. Gutierrez, *et al.*, Phys. Rev. Lett. **102**, 208102 (2009); M.H. Lee *et al.*, Phys. Rev. B **82**, 155455 (2010).

TT 16.3 Mon 18:45 HSZ 03

Conductance of DNA molecules: Effects of decoherence and bonding — ●MATÍAS ZILLY¹, ORSOLYA UJSÁGHY², and DIETRICH E. WOLF¹ — ¹Department of Physics and CeNIDE, University of Duisburg-Essen, 47048 Duisburg, Germany — ²Department of Theoretical Physics and Condensed Matter Research Group of the Hungarian Academy of Sciences, Budapest University of Technology and Economics, Budafoki út 8., 1521 Budapest, Hungary

The influence of decoherence and bonding on the linear conductance of single double-stranded DNA molecules is examined by fitting a phenomenological statistical model developed recently (Eur.Phys.J.B 68, 237 (2009)) to experimental results. The DNA molecule itself is described by a tight binding ladder model with parameters obtained from published ab initio calculations (J.Am.Chem.Soc. 127, 14894 (2005)). The good agreement with the experiments on sequence and length de-

pendence gives a hint on the nature of conduction in DNA and at the same time provides a crucial test of the model.

TT 16.4 Mon 19:00 HSZ 03

Electrostatic Potential Profiles and Current Voltage Characteristics of Molecular Wires: Effects of Dephasing — ●THOMAS STEGMANN, MATÍAS ZILLY, and DIETRICH E. WOLF — Department of Physics and CeNIDE, University of Duisburg-Essen, D-47048 Duisburg, Germany

The transport properties of molecular wires are studied using a tight-binding Hamiltonian and non-equilibrium Green's function (NEGF) method. We have developed a statistical model for the effects of dephasing [1], that assumes coherent transport between a distribution of completely phase randomizing regions. Recently, this model has been applied successfully on the conduction of DNA molecules in zero-bias approximation [2].

Here we present the extension of our model to finite bias requiring to take Coulomb interactions into account. This is done by means of the Hartree approximation where a self-consistent solution of both Poisson's equation and NEGF formalism has to be calculated. As a first application electrostatic potential profiles and current voltage characteristics of linear chains are shown. We demonstrate that the current depends sensitively on whether energy relaxation processes take place in the dephasing regions or not.

[1] M. Zilly, O. Ujsághy and D. E. Wolf, Eur. Phys. B, **68**:237 (2009)

[2] M. Zilly, O. Ujsághy and D. E. Wolf, Phys. Rev. B, **82**:125125 (2010)

TT 16.5 Mon 19:15 HSZ 03

Nonlinear effects of phonon fluctuations on transport through nanoscale junctions — ●DANIEL F. URBAN¹, REMI AVRILLER², and ALFREDO LEVY YEYATI² — ¹Physikalisches Institut, Albert-Ludwigs-Universität, 79104 Freiburg, Germany — ²Departamento de Física de la Materia Condensada C-XII, Universidad Autónoma de Madrid, E-28049, Madrid, Spain

We analyze the effect of electron-phonon coupling on the full counting statistics of a molecular junction beyond the lowest order perturbation theory. Our approach allows to take into account analytically the feedback between the non-equilibrium phonon and electronic distributions in the quantum regime. We show that for junctions with high transmission and relatively weak electron-phonon coupling this feedback gives rise to increasingly higher nonlinearities in the voltage dependence of the cumulants of the transmitted charges distribution.

[1] D. F. Urban, R. Avriller, and A. Levy Yeyati, Phys. Rev. B **82**, 121414 (R) (2010).

TT 16.6 Mon 19:30 HSZ 03

Statistical analysis of the thermopower of metallic atomic contacts — ●FABIAN PAULY¹, JUAN CARLOS CUEVAS², MARKUS DREHER³, PETER NIELABA³, and JANNE K. VILJAS⁴ — ¹Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology — ²Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid — ³Fachbereich Physik, University of Konstanz — ⁴Low Temperature Laboratory, Aalto University

We study theoretically the thermopower of Ag, Au, and Pt nanocontacts [1]. In our work, we employ classical molecular dynamics simulations to obtain structures during wire stretching and a tight-binding model for electric transport calculations. We find good agreement with experiment [2] for the evolution of the thermopower with increasing electrode separation and also the thermopower histograms. The comparison between the monovalent metals (Ag, Au) shows qualitative differences to those for multivalent ones (Pt).

[1] F. Pauly, J.C. Cuevas, M. Dreher, P. Nielaba, J.K. Viljas (in preparation)

[2] B. Ludoph and J. M. van Ruitenbeek, Phys. Rev. B **59**, 12290 (1999)