by the same strong disorder fixed point describing the onset of ferromagnetism in the random quantum Ising chain in a transverse field.

[1] A. Del Maestro, B. Rosenow, M. Müller, and S. Sachdev, Phys. Rev. Lett. **101**, 035701 (2008).

[2] J. A. Hoyos, C. Kotabage, and T. Vojta, Phys. Rev. Lett. **99**, 230601 (2007).

TT 22.12 Wed 12:45 HSZ 03

Quantum phase transitions in systems of coupled spin dimers — •Sandro Wenzel[1], Wolfhard Janke[1], and Stefan Wessel[2] — [1]Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04109 Leipzig — [2]Institut für Theoretische Physik III, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

We study quantum phase transitions in two-dimensional periodic arrangements of coupled spin-1/2 dimers, using a combination of quantum Monte Carlo simulations and effective field theories. Our numerical results on both ground-state properties and the finite-temperature scaling behavior in the quantum critical regime indicate, that depending on the spatial arrangement of the dimers, deviations occur to the scaling behavior of the three-dimensional Heisenberg universality class. We discuss the numerical evidence [1] for such unconventional quantum criticality, and possible relations to low-energy continuum theory beyond the conventional non-linear sigma model action.

[1] S. Wenzel, L. Bogacz, W. Janke, Phys. Rev. Lett. **101**, 127202 (2008).

TT 23: Transport: Nanoelectronics III - Molecular Electronics

Time: Wednesday 9:30–12:30 Location: HSZ 105

TT 23.1 Wed 9:30 HSZ 105

Length-dependent conductance and thermopower in single-molecule junctions of dithiolated oligophenylene derivatives: A density functional study — •Fabian Pauly[1,2], Janne Viljas[1,2], and Juan Carlos Cuevas[3] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, Germany — [2]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Germany — [3]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain

We study theoretically the length dependence of both conductance and thermopower in metal-molecule-metal junctions made up of dithiolated oligophenylenes contacted to gold electrodes [1]. We find that while the conductance decays exponentially with increasing molecular length, the thermopower increases linearly as suggested by recent experiments [2]. We also analyze how these transport properties can be tuned with methyl side groups. Our results can be explained by considering the level shifts due to their electron-donating character as well as the tilt-angle dependence of conductance and thermopower. Qualitative features of the substituent effects in our density functional calculations are explained using a tight-binding model. In addition, we observe symmetry-related even-odd transmission channel degeneracies as a function of molecular length.

[1] F. Pauly, J. K. Viljas, and J. C. Cuevas, Phys. Rev. B 78, 035315 (2008).

[2] P. Reddy, S.-Y. Jang, R. A. Segalman, and A. Majumdar, Science 315, 1568 (2007).

TT 23.2 Wed 9:45 HSZ 105

Opto-electronic properties of gold nanoparticle arrays — •Christoph Weiss, Markus A. Mangold, and Alexander W. Holleitner — Walter Schottky Institute, Technische Universität München, Am Coulombwall 3, 85748 Garching, Germany

The field of plasmonics has drawn a lot of interest in recent years. It deals with the interaction of metal clusters with light. Special attention was given to the fact that the exciting electric field is strongly enhanced at the surface of metal nanoparticles. Another topic where substantial research efforts are undertaken is the field of molecular electronics. Our research combines the two fields by examining the interaction of light with metal-molecule junctions. To this end, ordered hexagonal arrays of alkanethiol coated gold nanoparticles are produced by self-assembly. In such an array the nanoparticles are separated by nanometer-sized gaps. The nanoparticle arrays are manipulated with a focused ion beam and their opto-electronic properties are probed in the UV and visible spectrum. The strong plasmonic absorption of the nanoparticles can be readily observed in the photoresponse of arrays with alkanethiol coated gold nanoparticles.

We acknowledge the fruitful collaboration with J. Liao, M. Calame, C. Schönenberger, and the NCCR Nanoscience of the Swiss National Science Foundation (SNF) and thank for financial support by the DFG excellence initiative Nanosystems Initiative Munich (NIM).

TT 23.3 Wed 10:00 HSZ 105

Conductance of DNA molecular wires: bridging molecular dynamics and model Hamiltonians — •Benjamin Woiczikowski[2], Rafael Gutierrez[1], Rodrigo Caetano[1], Tomas Kubar[2], Marcus Elstner[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, D-01062 Dresden, Germany — [2]Institute for Physical and Theoretical Chemistry, Braunschweig University of Technology, D-38106 Braunschweig, Germany.

We present a hybrid method based on a combination of quantum/classical molecular dynamics (MD) simulations [1] and a model Hamiltonian approach to describe charge transport through biomolecular wires.[2] Our approach maps the molecular electronic structure (obtained from the MD simulations) onto a tight-binding model. The latter is then coupled to a bosonic bath which describes fluctuation effects from the solvent and from the conformational dynamics. We apply this approach to the case of pG-pC and pA-pT oligomers as typical cases. We show that conformational fluctuations are crucial in determining charge transport. Especially, our results indicate that pA-pT shows a much larger current than pG-pC, in contrast to transport calculations performed on static configurations.

[1] T. Kubar, P. B. Woiczikowski, G. Cuniberti, and M. Elstner, J. Phys. Chem. B 112, 7937 (2008).

[2] R. Gutierrez, R. Caetano, B. Woiczikowski, T. Kubar, M. Elstner, and G. Cuniberti, submitted (2008).

TT 23.4 Wed 10:15 HSZ 105

Screw motion of a DNA duplex during translocation through a nanopore: A coarse-grained model — •Rafael Gutierrez[1], Jewgeni Starikov[2], Dirk Hennig[3], Hiroaki Yamada[4], Gianaurelio Cuniberti[1], and Bengt Norden[5] — [1]Institute for Materials Science, Dresden University of Technology, D-01062 Dresden, Germany — [2]Institute for Theoretical Solid State Physics, University of Karlsruhe, D-76131 Karlsruhe, Germany — [3]Institute for Physics, Humboldt University of Berlin, D-12489 Berlin, Germany — [4]Yamada Physics Research Laboratory, Niigata 950-2002, Japan — [5]Department of Physical Chemistry, Chalmers University of Technology, SE-412 96, Gothenburg, Sweden

Based upon the structural properties of DNA and their counterion-water surrounding in solution, we have introduced a screw model describing DNA translocation through artificial nanopores in a qualitatively correct way.[1] This model represents DNA as a "screw", whereas the counterion-hydration shell is a "nut". When an electrical potential is applied across a membrane with a nanopore, the "screw" and "nut" begin to move with respect to each other, so that their mutual rotation is coupled with their mutual translation. As a result, there are peaks of electrical current connected with the mutual translocation of DNA and its counterion-hydration shell, if DNA has some non-regular base-pair sequence. The calculated peaks of current strongly resemble those observed in the pertinent experiments.

[1] E. B. Starikov, D. Hennig, H. Yamada, R. Gutierrez, G. Cuniberti, and B. Norden, submitted (2008)

TT 23.5 Wed 10:30 HSZ 105

Charge-memory polaron effect in molecular junctions — •Dmitry A. Ryndyk[1], Pino D'Amico[1], Gianaurelio Cuniberti[2], and Klaus Richter[1] — [1]Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany — [2]Institute for Material Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, D-01062 Dresden

The charge-memory effect, bistability and switching between charged and neutral states of a molecular junction, as observed in recent STM