DY 21: Thermodynamics and Statistical Physics of Small Systems (contributed talks)

Time: Wednesday 11:45–13:15 Location: HÜL 186

DY 21.1 Wed 11:45 HÜL 186

Stochastic energetics of the Büttiker-Landauer Brownian Motor and Refrigerator — •Ronald Benjamin — German Aerospace Center, Cologne, Germany

The energetics of a Brownian motor and refrigerator driven by position dependent temperature, known as the Büttiker-Landauer motor and refrigerator, is investigated by extensive numerical simulations of the inertial Langevin equation. We identify parameter values for optimal performance of the motor and refrigerator. Inertial effects strongly affect the thermodynamic behavior of the system even in the overdamped limit. The behavior of the motor and refrigerator, in the linear response regime, is examined under finite time conditions and we find that the efficiency can never reach that of an endoreversible engine working under the same condition. Finally, we investigate the role of different potential and temperature profiles to enhance the efficiency of the system. Our simulations show that optimizing the potential and temperature profile leads only to a marginal enhancement of the system performance and the reasons for this are given.

DY 21.2 Wed 12:00 HÜL 186

Measurements in optimal finite-time thermodynamics — •David Abreu and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

The second law states the impossibility of extracting work from a system in a single thermal bath. However, as Sagawa and Ueda recently showed [1], this becomes possible if we extract information out of the system through measurements. We show here a basic example of an isothermal engine based on the conversion of information into work.

Our model system consists in a Brownian particle confined in a harmonic potential that we want to displace from its initial position to a fixed final position in finite time. Performing one or more measurements of the position of the particle at the beginning or during the process leads to work extraction from the thermal bath. We optimize the output work of such a process and build a cyclic engine based on it. We observe the presence of an optimal cycle-time which depends on the precision of the measurements.

We then quantify the information obtained during the measurements and show that we can transform it all into useful work in the quasistatic limit, given that we control not only the position but also the stiffness of the potential. We compare this result to a discrete two-level system, analogous to the Szilard engine, and show that the expressions of the total extractable work in both cases are similar and consistent with each other.

[1] T. Sagawa and M. Ueda. Phys. Rev. Lett. 104, 090602 (2010).

DY 21.3 Wed 12:15 HÜL 186

Free gold clusters in CO and O_2 atmosphere: an ab initio study. — •Elizabeth C. Beret, Luca M. Ghiringhelli, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft Berlin, Germany

The marked catalytic activity of gold nanoparticles has inspired a large number of scientific contributions from different fields. However, many questions still lack a satisfying answer, for example what are the structures and stoichiometries of the gold particles in the presence of the reactive gases, and how do their catalytic properties depend on the particle size [1].

We answer these questions for neutral gold clusters modeled in a gas phase atmosphere containing CO and O_2 in variable compositions, and in a temperature range between 100 and 600 K. To this aim, DFT (PBE)–based *ab initio atomistic thermodynamics* technique [2] is applied, including full account of the vibrational contribution to the free energy. As a result, the preferred cluster+adsorbate structures for different environmental conditions are obtained and interpreted as candidate intermediates in the catalytic CO oxidation reaction.

[1] R. Meyer, C. Lemire, S. K. Shaikhutdinov and H. J. Freund, *Gold Bull.* **2004**, *37*, 72–124. [2] K. Reuter and M. Scheffler, *Phys. Rev. B* **2001**, *65*, 035406; C. M. Weinert and M. Scheffler, *Mat. Sci. Forum* **1986**, **10–12**, 25–30; M. Scheffler and J. Dabrowski, *Phil. Mag. A* **1988**, *58*, 107–121.

DY 21.4 Wed 12:30 HÜL 186

Interaction effects and performance of a photoelectric device — Marcel Dierl[1,2] and •Mario Einax[1,2] — [1]Institut für Physik, Technische Universität Ilmenau, 98684 Ilmenau, Germany — [2]Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49076 Osnabrück, Germany

We investigate a one-dimensional photoelectric device, where charge carriers interact via coupling constant V. Based on classical time-dependent density functional theory calculations, we find that nearest-neighbor interactions are of crucial importance for the current, the power as well as the efficiency of the nano-device. To point out the validity of this analytical approach, kinetic Monte Carlo simulations are performed.

DY 21.5 Wed 12:45 HÜL 186

Kramers barrier crossing as a cooling machine — •Philip Schiff and Abraham Nitzan — School of Chemistry, Tel Aviv University, Israel

The achievement of local cooling is a prominent goal in the design of functional transport nanojunctions. One generic mechanism for local cooling is driving a system through a local uphill potential step. In this talk we examine the manifestation of this mechanism in the context of the Kramers barrier crossing problem. For a particle crossing a barrier, the local effective temperature and the local energy exchange with the thermal environment are calculated, and the coefficient of performance of the ensuing cooling process are evaluated. These results represent a heuristic demonstration of a mechanism for pumping heat in a nanosystem.

DY 21.6 Wed 13:00 HÜL 186

Effects of polymer grafting on the thermodynamic equilibrium behavior of single polymer adsorption — •Monika Möddel[1], Wolfhard Janke[1], and Michael Bachmann[2] — [1]Institut für Theoretische Physik, Universität Leipzig — [2]Institut für Festkörperforschung, Theorie II, Forschungszentrum Jülich

The adsorption of single polymers onto flat attractive substrates has been the subject of several studies in the past. Especially for numerical studies of finite chains it is popular to consider the chain to be grafted, i.e. permanently attached to the substrate at one end. Compared to non-grafted polymer adsorption, translational entropy is strongly suppressed, and thus the phase space lacks completely desorbed conformations some distance away from the substrate. We systematically show how the competition between translational and conformational entropies changes the character of the adsorption transition. We present a comparison of the thermodynamic behavior of free and grafted chains for a range of different surface attraction strengths and temperatures. This is done by parallel tempering simulations of an off-lattice coarse-grained homopolymer [1] and a combined canonical and microcanonical analysis of energetic and steric observables.

[1] M. Möddel, M. Bachmann, and W. Janke, J. Phys. Chem. B 113, 3314 (2009); M. Möddel, W. Janke, and M. Bachmann, Phys. Chem. Chem. Phys. 12, 11548 (2010).