DY 57: Poster - Diffusion

Brownian Motion and Transport; Reaction-Diffusion Systems; Anomalous Diffusion; Brownian Motion and Transport; Microswimmers

Time: Thursday 16:00–18:00 Location: Poster A

DY 57.1 Thu 16:00 Poster A

Mobility of colloids driven through a permeable corrugated channel — •Konstantin Zak, Robert Gernert, and Sabine H. L. Klapp — Institut für theoretische Physik, Technische Universität Berlin

Nonequilibrium transport of colloidal suspensions is an active field of research – even for the paradigmatic model of effectively one-dimensional flow through a channel with a corrugated confinement. Here we consider a non-perfect confinement where the particles may escape from the system and enter to it. This permeable confinement is modelled via a high energetic barrier between the channel and a particle bath with constant density. For the theoretical description of the overdamped, effectively one-dimensional flow of hard spheres through the channel we employ the Dynamical Density Functional Theory (DDFT). The influence of the system-bath interaction is studied in terms of mobility and density distribution of the colloids in flow direction. We also present first results concerning the generalisation of the system towards two dimensions.

DY 57.2 Thu 16:00 Poster A

A Lattice Monte Carlo Battery Model — •Oliver Rubner, Volker Lesch, Linus Scholz, and Andreas Heuer — Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster

The theoretical simulation of Li-Ion batteries is an essential tool for the understandig of the complex processes that take place in electrodes as well as in electrolytes. Many models exist that focus on molecular details involving quantum chemical, molecular dynamics or continuum Monte Carlo calculations on the one hand and continuum models that treat a battery cell as a whole system on the other hand. We want to bridge the gap between these approaches by presenting a lattice Monte Carlo model that uses molecular and macroscopic parameters provided by experiments or these aforementioned techniques. We show how the influence of molecular parameters like interaction energies on cell properties like voltage and capacity can be determined in this simplified model and how it can be used to understand some of the basic principles of Li-batteries.

DY 57.3 Thu 16:00 Poster A

Thermal conductivity and self-diffusion coefficients for the TIP4P/2005 water model over a wide range of thermodynamic conditions — •Sven Engelmann and Reinhard Hentschke — Bergische Universität, 42279 Wuppertal, Germany

Using the Molecular Dynamics simulation technique we compute thermal conductivity and self-diffusion coefficients for the TIP4P/2005 water model together with a number of other thermodynamic quantities. The transport coefficients are obtained using the attendant Green-Kubo relations applied to equilibrium trajectories. The thermodynamic conditions include the saturation line in the temperature range from 273K to 373K. In addition we obtain results along two isotherms at 300K and 400K for pressures ranging from about 10 bar to 10 kbar and along an isobar at 1 bar covering again the above temperature range. The simulation data are compared to experimental measurements as well as to previous simulation results obtained with a number of other methods including also other water models. We present a critical evaluation of all simulation results in relation to the different thermodynamic conditions.

DY 57.4 Thu 16:00 Poster A

A coupled Molecular Dynamics / kinetic Monte Carlo Approach for Protonation Dynamics in Extended Systems — •Gabriel Kabbe[1], Christian Dressler[1], Christoph Wehmeyer[2], and Daniel Sebastiani[1] — [1]Department of Chemistry, Martin-Luther Universität, Halle-Wittenberg, von-Danckelmann-Platz 4, 06120 Halle/Saale, Germany — [2]Institute of Mathematics, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

We propose a multi-scale simulation scheme that combines first-principles Molecular Dynamics (MD) and kinetic Monte Carlo (kMC) simulations to describe ion transport processes. On the one hand, the molecular dynamics trajectory provides an accurate atomistic structure and its temporal evolution, and on the other hand, the Monte Carlo part models the long-time motion of the acidic protons. Our hybrid approach defines a coupling scheme between the MD and kMC simulations that allows the kMC topology to adapt continuously to the propagating atomistic microstructure of the system. We exemplify the performance of our MD/kMC model on the basis of various proton conducting molecular systems.

DY 57.5 Thu 16:00 Poster A

Excited State Proton Transfer in Aqueous Media: Ab-Initio Molecular Dynamics Simulation of Photoacids — •Gül Bekcioglu, Felix Hoffmann, and Daniel Sebastiani — Martin-Luther-Universität Halle-Wittenberg, Institut für Chemie - Theoretische Chemie

Photoacids are molecules which undergo a decrease in pKa value upon photoexcitation.[1,2] Since their acidity can be controlled in a very defined manner they are important model system for the investigation of proton transport in aqueous media. However, many details of the proton transfer from the photoacid to water remain elusive, for example, the structure and stability of the contact ion pair between the photoacid and the hydrated proton. A particular drastic drop in pKa value is exhibited by the "super" photoacid N-methyl-6-hydroxyquinolinium (HMQ). [3] Here, we present a microscopic study of the role water plays in mediating excited state proton transfer of HMQ in aqueous solution. The central question addressed here is the determination of elementary steps that lead to a full dissociation of the proton. In this regard, we computed IR spectra from Wannier center calculations to elucidate spectroscopic fingerprints of specific intermediates during the acid dissociation. [3]

[1] G. Bekcioglu, C. Allolio, M. Ekimova, E. T. J. Nibbering, and D. Sebastiani, Phys. Chem. Chem. Phys.,16, 13047-13051, (2014)

[2] G. Bekcioglu, C. Allolio, and D. Sebastiani, Phys. Chem. Chem. Phys., Submitted, (2014)

[3] G. Bekcioglu, F. Hoffmann, and D. Sebastiani, in preparation.

DY 57.6 Thu 16:00 Poster A

Bifurcations in two-dimensional oscillator arrays: numerical study — •Claudia Lenk and J. Michael Köhler — Institut für Chemie und Biotechnologie, TU Ilmenau, Ilmenau, Deutschland

In the range of critical coupling strength bifurcations arise in arrays of locally coupled nonlinear oscillators. Thereby, interesting effects as amplitude modulations, multiperiode oscillations and burst patterns occur, which are similar to patterns observed in neuronal networks or in the heart. We study the occurrence of bifurcations and special patterns by calculations of the Fitzhugh-Nagumo equations of a catalyst distribution in form of a micro spot pattern. Its dependence on spot size, spot distance, spot shape and parameter variations will be discussed. The importance of gradients of spot distance or spot size for the appearance of bifurcations will be shown. Furthermore, we study the influence of the dimensionality of the oscillator arrays and the introduction of defects in the oscillator arrays for arisal of burst and other special patterns.

DY 57.7 Thu 16:00 Poster A

From integrated Brownian motion to Lévy walks — •Tony Albers and Günter Radons — Technische Universität Chemnitz, Germany

In a recent publication [1], we investigated the weakly nonergodic behavior of integrated Brownian motion. In this contribution, we will show how integrated Brownian motion can be mapped to a continuous time random walk with a spatiotemporal coupling of the form $\psi(x,t) \propto \delta(|x| - t^{3/2})t^{-3/2}$, where $\psi(x,t)$ describes the probability for the occurrence of a waiting time of duration t followed by a jump of length x. We investigate the nonergodic behavior of this Lévy walk by contrasting the time dependence of the ensemble-averaged and the time-averaged mean-squared displacement (MSD) and analyzing the random nature of the latter. Moreover, all quantities are studied in dependence on the ageing time which is the elapsed time between the beginning of the process and the beginning of the measurement. We

compare our findings with the results obtained for integrated Brownian motion and discuss the similarities and differences.
[1] Tony Albers and Günter Radons, Phys. Rev. Lett. **113**, 184101 (2014)

DY 57.8 Thu 16:00 Poster A

Non-adiabatic quantum pumping by a randomly moving potential barrier — Stanislav Dervyanko[1] and •Daniel Waltner[2] — [1]Department of Physics of Complex Systems, Weizmann Institute of Science, Rehovot 76100, Israel — [2]Fakultät für Physik, Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg

We look at random AC fluctuations of the electrical charge in an open 1D quantum system where the potential barrier experiences random lateral motion in time. Our treatment is essentially non-adiabatic. Both diffusive and ballistic (Lévy) regimes are considered. For a finite size system the probability current as well as the net accumulated electric charge experience random fluctuations over the static background. We show that in the large-time limit $t \to \infty$ the wavefunction is naturally separated into the Berry-phase component (resulting from the singular part of the wave amplitude in the co-moving frame) and the non-adiabatic correction (arising from fast oscillating, slow decaying tails of the same amplitude). In the special limit of delta-correlated continuous Gaussian random walk we obtain a closed analytical expressions for the ensemble averaged amplitude in the co-moving frame and demonstrate that the main contribution to the average wavefunction and probability current comes from the Berry-phase component.

DY 57.9 Thu 16:00 Poster A

Simulation of Anomalous Transport in Model Crowded Media — •Markus Spanner[1], Felix Höfling[2], Gerd E. Schröder-Turk[1], and Thomas Franosch[3] — [1]Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]MPI für komplexe Systeme and IV. Institut für Theoretische Physik, Universität Stuttgart, Germany — [3]Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, Austria

We study large-scale computer simulations of particles in 2d and 3d dense-packed porous systems. Subdiffusive dynamics $\delta r^2(t) \sim t^{2/z}, z > 2$ can be observed at a critical obstacle density, when the tracer particle can barely squeeze through between the host structure.

Starting from the Lorentz model, which simply consists of a point-like tracer moving through an array of random overlapping spheres, we modify a number of simulation details (tracer dynamics, obstacle distribution, introduction of an external force) one at a time – from most simple towards more realistic porous systems. By extracting critical exponents of the dynamics in these systems, we gain a better understanding of the universal or non-universal nature of the observed exponents.

DY 57.10 Thu 16:00 Poster A

Active Brownian micro-swimmers in viscoelastic media — •Juan Ruben Gomez Solano[1,2] and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universitaet Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Max-Planck-Institute for Intelligent Systems, Heisenbergstrasse 3, 70569 Stuttgart, Germany

The motion of many natural micro-swimmers, such as bacteria and spermatozoa, commonly takes place in viscoelastic fluids or in complex crowded environments. The understanding of their swimming mechanisms has triggered a lot of experimental and theoretical work in recent years as well as the development of artificial self-propelled macro- and micro-swimmers. Although the motion of artificial swimmers in Newtonian fluids has been extensively studied, only few works have focused on active swimmers in viscoelastic media. In this work, we experimentally investigate the motion of spherical Janus particles in a critical binary viscoelastic fluid. The particles are self-propelled by local demixing of the fluid induced by laser illumination. We find that, unlike active Brownian motion in a Newtonian fluid, the rotational diffusion coefficient of a particle moving in a viscoelastic fluid dramatically increases with increasing particle velocity. This gives rise to a significant increase of the effective translational diffusion coefficient of the active particles with increasing laser illumination compared to the Newtonian case, which can be interpreted as an enhanced micro-swimming mechanism.

DY 57.11 Thu 16:00 Poster A

Lane formation in a two dimensional system with Lennard-Jones like interactions — •Christopher Wächtler, Florian Kogler, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Using Brownian Dynamics simulations we investigate a prototype model system undergoing lane formation. The latter is a non-equilibrium transition in binary mixtures of oppositely driven particle species. In contrast to previous studies of repulsively interacting particles, which form perfect lanes only at infinitely large driving forces [1], we here examine this transition in a system involving attractive Lennard-Jones like interactions. We present new findings on how parameters such as system size, driving force and interaction strength influence lane formation in this system.
[1] T. Glanz, H. Löwen, J. Phys. Condens. Matter 24, 464114 (2012)

DY 57.12 Thu 16:00 Poster A

Numerical investigation of droplets driven by Marangoni flow — •Laura Stricker, Juergen Vollmer, and Stephan Herminghaus — Max Planck Institute for Dynamics and Self-Organization (MPI-DS), Goettingen, Germany

The motion of artificial microswimmers can strikingly resemble collective motion in biological systems even though it only involves physical and chemical processes. A detailed understanding of their emergent swarming properties may therefore help to distinguish merely physics-related from biology-related aspects of motion in biological systems. In the present work, we focus on modelling a new type of artificial microswimmers, where propulsion is achieved by Marangoni flow. In particular, we characterize the parametric dependence of the motion and we address the propulsion mechanism. In order to do so, we developed a flexible CFD model based on a level set method, easily adaptable to different kinds of swimmers. We derived the flow field inside and outside individual droplets, and took into account the two-way coupling of the swimmers motion and the external flow. This allowed us to explore the dependence of propulsion on experimentally tunable parameters, like the droplet size and surfactant concentration. Future extensions of the present work will include the interactions between small numbers of swimmers, and the collective behavior of large assemblies, in the framework of a full multiscale approach

DY 57.13 Thu 16:00 Poster A

Active particles in inhomogeneous environments — •Kevin Schröer, Martin P. Magiera, and Lothar Brendel — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE), University of Duisburg-Essen, D-47047 Duisburg, Germany

Recent molecular dynamics simulations of dense suspensions of self-propelled Brownian spheres show the appearance of self-organized patterns, large-scale collective motion and phase separation via particle agglomeration [1].

In addition to that we follow the idea of an environment-dependent propulsion mechanism by introducing "passivity"-areas in which the propulsion of the particles is suppressed. Accumulation-effects are observed in and around these areas which serve as accumulation-nuclei. The swimmers are modeled in 2D and 3D via Langevin-Dynamics in order to include inertial effects and to reevaluate the latter's importance for the accumulation process. Further investigations focus on the question to which extent hydrodynamic interactions play a role in the particle interplay and the collective behavior.

References:
[1] A. Wysocki, R.G. Winkler, G. Gompper, EPL 105, 48004 (2014)

DY 57.14 Thu 16:00 Poster A

Active microrheology of dense microswimmer suspensions — •Alexander Liluashvili and Thomas Voigtmann — DLR, Köln, Deutschland

The dynamics of self-propelled particles like microswimmers in dense environments are studied using the mode coupling theory of the glass transition. The theory is developed to investigate the glassy dynamics of active suspensions out-of-equilibrium, violating the fluctuation-dissipation-theorem relations.

As a starting point of mathematical calculations the Mori-Zwanzig equations with orientational degrees of freedom in two dimensions are used. The final equations for the density two-point function and the friction coefficient in the time domain are solved numerically in a schematic model including the orientational degrees of freedom, but neglecting the spatial fluctuations.

DY 57.15 Thu 16:00 Poster A

Soft Elastic Capsules in Axisymmetric Linearized Viscous Flow — •Horst-Holger Boltz and Jan Kierfeld — TU Dortmund, Dortmund, Germany

We present an iterative solution scheme to find the stationary shape of a deformable axisymmetric elastic surface moving at very low Reynolds numbers. We use this to study the sedimentation of soft elastic capsules with Hookean stretching and bending energies.

DY 57.16 Thu 16:00 Poster A

How fast is a magnetic snail creeping down a hill? — •Anita Freundorfer, Stefan Hartung, Ingo Rehberg, and Reinhard Richter — Experimentalphysik 5, Universität Bayreuth, D-95440 Bayreuth, Germany

We investigate a permanent magnet floating on a drop of ferrofluid, which is positioned at the upper most end of an inclined plane of perspex. Releasing a trigger the magnet travels down the ramp leaving a trace of ferrofluid behind. For different angles of inclination α of the plane we record the time dependent position $x_\alpha(t)$ of the magnet and determine its velocity $v_\alpha(t) = dx_\alpha(t)/dt$. The latter depends on the thickness $h_\alpha(t)$ of the ferrofluidic film which is measured by means of light absorption. For a specific time we plot the layer thickness $h_\alpha(t)$ versus the capillary number $Ca = \frac{\eta \cdot v}{\sigma}$ where η denotes the viscosity and σ the surface tension. In the regime $Ca < 0.01$ we find $h \propto C_a^{2/3}$, whereas for $Ca > 0.01$ the scaling $h \propto a \cdot C_a^{1/2}$ is confirmed. These scaling laws for the film thickness are in accordance with those found for a vertical plate pulled out of a liquid [1]. After the magnet arrives at the bottom of the plane the latter is switched to $\alpha = 0$. The magnet creeps back on its trace, up to the end, like an inverse snail absorbing its own slime, which is also investigated quantitatively.

[1] S. Weinstein, K. Ruschak, *Annu. Rev. Fluid. Mech.* vol.76, 066301 (2004).