DY 4: Statistical Physics (general) II

Time: Monday 14:00–16:00 Location: H47

DY 4.1 Mon 14:00 H47

Naproxen particle by RESS: A molecular dynamic study. — •Frank Römer and Thomas Kraska — University of Cologne, Department of Chemistry, Luxemburger Straße 116, D-50939 Köln

With a recently developed method (*J. Phys. Chem. C* **113**, 19028-19038, 2009) we study the formation of Naproxen particles by expansion of a supercritical solution (RESS) by means of molecular dynamics simulation. For this investigation we propose a new potential model for Naproxen. The employed van der Waals parameters are based on the TraPPE model. The charges and intramolecular interactions due to internal degrees of freedom are obtained from *ab initio* calculations. We analyze the bulk properties of the Naproxen model as well as those of small particles. The expansion path of a Naproxen/CO_2 solution is compared to the napthalene/CO_2 system. For a wide range of pre-expansion conditions (310 K - 400 K) we determine the nucleation rates and compare them to calculations with the the classical nucleation theory.

DY 4.2 Mon 14:15 H47

Molecular dynamics simulation of nucleation in binary systems — •Stephan Braun and Thomas Kraska — University of Cologne, Department of Chemistry, Luxemburger Str. 116, D-50939 Köln

The vapour-liquid nucleation of the binary system n-nonane/methane is investigated by molecular dynamics simulation. The supersaturation of the system is achieved by cooling down the system during expansion in order to closely mimic the real process which is for example applied in practice to separate heavy compounds from natural gas.

The expansion is simulated via a stepwise enlargement of the simulation box with short equilibration runs in between. From these simulations one obtains several details of the nucleation process, which are difficult or impossible to obtain from experiments. These are the early stages of nucleation and growth taking place on the nanosecond time scale. The simulations provide information on the way how binary supercritical systems nucleate on the molecular scale as well as on nucleation rates and critical cluster sizes. Since the n-nonane clusters contains a large amount of methane molecules the composition of the clusters is analysed with respect to the mole fractions to get a better understanding of the properties of the clusters.

DY 4.3 Mon 14:30 H47

Size Distribution and Correlation Functions of Hanging Dew Droplets — •Tobias Lapp[1], Johannes Blaschke[1], Andrew Scullion[2], Jürgen Vollmer[1], and Björn Hof[1] — [1]MPI for Dynamics and Self-Organization, 37073 Göttingen, Germany — [2]Carleton University, Ottawa, Ontario K1S 5B6

The formation, growth and coarsening of dew droplets on flat surfaces has widely been studied in the physics literature under the keyword "Breath Figures". As an experimental setup we built a vapor chamber not too dissimilar to a steam cooker: A cell with water is heated from below. The water partially evaporates and condenses on a cooled ceiling plate. Applying a dark field illumination technique yields high resolution images of the droplets that we analyze to measure the droplet size distribution and the pair correlation function of droplets.

We compare the experimental data to numerical simulations to investigate how the interplay of coalescence and dripping of droplets yields locally correlated droplet patterns. Moreover, we use the pair correlation function to formulate a Boltzmann equation for the evolution of the size distribution.

DY 4.4 Mon 14:45 H47

Particle density distributions in hard sphere crystals — •Stefan Görig and Martin Oettel — Jo-Gu Uni Mainz, Deutschland

We discuss the shape of the density profiles around the fcc lattice sites in hard sphere crystals with bulk packing fractions near coexistence. Monte Carlo results for the peak width and the anisotropy are compared with results from density functional theory (DFT) using fundamental measure functionals. Crystal free energies computed with a novel simulation method agree well with the corresponding DFT results. Furthermore we discuss the applicability of the phase field crystal ansatz (using a local free energy density) to the hard sphere system in view of further applications for nucleation and growth processes.

DY 4.5 Mon 15:00 H47

Randomly driven hysteresis — •Sven Schubert and Günter Radons — Chemnitz University of Technology, D-09107 Chemnitz

Many physical and technical systems are characterized by non-trivial hysteretic behavior. Topical examples are porous materials, shape memory alloys, and magnetic nanoparticles. The fact that external fields are often entirely erratic leads to the question how hysteretic systems respond to random processes. Hence we are interested in autocorrelation or spectral properties, respectively, of Preisach hysteresis models driven by stochastic input scenarios.

Starting from a known scenario, the case of uncorrelated input signals, where long-term correlations and $1/f$-noise could emerge due to hysteresis [1], we investigate the role of long-term correlations in input signals for hysteretic systems using numerical simulations. For systematic investigations, firstly, we establish a method to compute correlated input processes that allows us to determine the probability density and long-term autocorrelation decay of the input signal. Secondly, different hysteresis outputs are computed and, lastly, their correlation decay is analyzed.

Our investigation indicates that correlations in the input signal compete with hysteretically induced correlations. This results in two regimes: (1) long-time tails of input correlation survive in the output correlation or (2) we observe long-time tails due to hysteresis, as if they were induced by δ-correlated input. In the latter case long-term correlations due to hysteresis cover faster decaying input correlations.

[1] G. Radons, Phys. Rev. Lett. **100**, 240602 (2008).

DY 4.6 Mon 15:15 H47

Phase space master equations for the Lipkin-Meshkov Hamiltonian — •Bernard P.J. Mulligan[1], William T. Coffey[2], Yuri P. Kalmykov[3], and Serguey V. Titov[4] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Trinity College Dublin, Ireland — [3]Universite de Perpignan, France — [4]Russian Academy of Sciences, Russia

The spin system with the Lipkin-Meshkov Hamiltonian

$$\beta\hat{H}_S = -\xi\hat{S}_X - \sigma\hat{S}_Z^2$$

(ξ and σ are external and internal field parameters) is treated as a nonaxially symmetric example of the phase space description of spin dynamics using a master equation for the quasiprobability distribution function of spin orientations in the representation (phase) space of the polar angles (analogous to the Wigner phase space distribution for translational motion). The master equation yields (via the Wigner-Stratonovich transformation of the density matrix) the solution as a Fourier series in the spherical harmonics with Fourier coefficients given by the statistical moments in a manner analogous to the classical distribution. In particular we take the values of S = 1/2,1.

DY 4.7 Mon 15:30 H47

Investigation of multidisperse packing problems in higher dimensions — •Andre Müller, Sebiha Sahin, Elmar Schömer, and Johannes J. Schneider — Center for Computational Research Methods in Natural Sciences, Johannes Gutenberg University of Mainz, Staudinger Weg 7, 55099 Mainz, Germany

Recently, a benchmark contest was performed in which a multidisperse system of hard disks with different integer radii $r_i = i$, $i = 1, \ldots, N$ had to be packed in a circular environment in the way that the radius of the circumcircle around these disks is minimized. With our packing algorithm, which was rated by the Time Magazine as one of the 50 best inventions of the year 2009, we were able to match and beat all world records established during the contest. Now we extend our approach to higher dimensions $D \geq 3$ and present results for the dynamics of the optimization process, the scaling laws for optimum values, and the properties of quasioptimum solutions.

DY 4.8 Mon 15:45 H47

Effect of critical adsorption of binary solvent on distribution of ionic solute near a charged surface. — •Anna Maciolek[1,2] and Alina Ciach[1] — [1]Max-Planck Institut fuer Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — [2]Institute of Physical Chemistry of Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warszawa,

Poland

We study near-critical binary mixtures containing ionic solutes near a charged wall preferentially adsorbing one component of the solvent. Within a Landau-Ginzburg approach extended to include electrostatic interactions and the chemical preference of ions for one component of the solvent, we find that critical adsorption changes significantly distribution of ions near the wall. This may have important implications in confining geometries, in particular, for an electrostatic interactions of colloids in a binary near-critical solvent.