DY 82: Glasses and Glass Transition (joint session DY/CPP)

Time: Friday 10:00–12:45 Location: BH-N 334

DY 82.1 Fri 10:00 BH-N 334

Can the glass transition occur in non-equilibrium? — •Michael Schmiedeberg — Institut für Theoretische Physik 1, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Recently, there have been great advances in the simulation of equilibrated hard sphere systems up to high densities that can even exceed the athermal jamming packing fraction (see, e.g., [1]). As a consequence, several researchers claim that all previous simulations were obsolete and that it even was not allowed to do further studies of non-equilibrium systems.

In my contribution I want to motivate that by limiting the research to systems in equilibrium one misses important and interesting phenomena that exist in non-equilibrium systems, e.g., ageing, avoidance of crystallization, history-dependence, as well as many other properties of the dynamical glass transition and of glasses. I argue that dynamical glasses obtained by rapid quenches can be significantly different from ideal, structural glasses that might occur in equilibrated systems.

[1] A. Ninarello, L. Berthier, and D. Coslovich, Phys. Rev. X 7, 021039 (2017).

DY 82.2 Fri 10:15 BH-N 334

Nonlinear response theory: simple stochastic models — •Gregor Diezemann — Institut für Physikalische Chemie, Universität Mainz

The effect of large electric fields on the relaxation of supercooled liquids and also other systems like ionic liquids and crystals has been studied intensively during the last decade. Due to the formal lack of an analogue to the well known fluctuation dissipation theorem valid for linear response, one essentially relies on model calculations in the nonlinear case. There are a number of different models that have been used to compute the nonlinear response of glassforming systems, such as the so-called box model, the model of isotropic dipole reorientations or the dipole flips in an asymmetric double well potential (ADWP). I will discuss the results of model calculations of the nonlinear response for simple stochastic models for the dynamics. In particular, I will consider the ADWP model which is known to exhibit a peak in the modulus of the third-order response in a narrow temperature range around some characteristic temperature. Interestingly, in fifth order one observes peaks in the modulus around two characteristic temperatures. These peaks are related to the vanishing of the nonlinear static susceptibility in the respective order. The results will be discussed in the light of recent experimental observations.

DY 82.3 Fri 10:30 BH-N 334

Lokaler Debye-Prozess? Einblicke in 1-Propanol mit Hilfe der Triplett-Solvatationsdynamik — •Daniel Koestel[1], Peter Weigl[2], Thomas Blochowicz[2] und Thomas Walther[1] — [1]TU Darmstadt, Institut für Angewandte Physik — [2]TU Darmstadt, Institut für Festkörperphysik

Mit Hilfe der Triplett-Solvatationsdynamik (TSD) ist es möglich das Relaxationsverhalten unterkühlter Flüssigkeiten und auch in geometrisch eingeschränkten Systemen lokal zu untersuchen [1]. Dabei wird ein Farbstoff in geringer Konzentration in der Probe gelöst und mittels eines UV-Laserpulses in einen langlebigen Triplett-Zustand angeregt. Durch die Relaxation der den Farbstoff umgebenden Moleküle kommt es zu einer Rotverschiebung des vom Farbstoff emittierten Spektrums. Diese zeitabhängige Stokes-Verschiebung kann zur Bestimmung des lokalen Relaxationsverhaltens der Solvationshülle genutzt werden [1]. Wasserstoffbrückenbildende Flüssigkeiten sind von besonderem Interesse, da diese auch in biologischen Systemen eine zentrale Rolle einnehmen. Besonders Monohydroxy Alkohole weisen dabei in der dielektrischen Spektroskopie den prominenten Debye-Prozess auf [2], dessen mikroskopischer Ursprung nach wie vor Gegenstand kontroverser Diskussion ist und meist der Relaxation einer transienten, supermolekularen Kettenstruktur zugeschrieben wird, die sich aufgrund von Wasserstoffbrücken ausbildet [3]. Dabei gehen wir der Frage nach, ob und wie diese Kettendynamik von einer lokalen Sonde detektiert wird.

[1] R. Richert. J. Chem. Phys. 113 (2000) [2] J. Gabriel et al. J. Phys. Chem. B 121 (2014) [3] R. Böhmer et al. Phys. Rep. 545 (2014)

DY 82.4 Fri 10:45 BH-N 334

DY 82.4 Fri 10:45 BH-N 334

Analytical solution of the spin model on the Bethe lattice — •Koray Önder[1,2], Till Kranz[1,2], and Matthias Sperl[1,2] — [1]Institut für Theoretische Physik, Uni Köln — [2]Institut für Materialphysik im Weltraum, DLR Köln

The cooperative facilitation scenario (CFS) on the Bethe lattice shows similarities in the correlation functions with the mode coupling theory (MCT). The first studies by fitting some critical exponents on the CFS are in good agreement with the MCT predictions [1].

The fact that the CFS on the Bethe lattice yields a bifurcation scenario can be used to describe the asymptotic dynamics of the system. As a result we obtain analyticaly exact predictions for the critical exponents and the master function.
[1] M. Sellitto, Phys. Rev. Lett. **115**, 225701 (2015)

DY 82.5 Fri 11:00 BH-N 334

Structure and dynamics of water-like models — •Robin Horstmann and Michael Vogel — Institut für Festkörperphysik, TU Darmstadt, Hochschulstraße 6, 64289 Darmstadt, Germany

Among glass-forming liquids tetrahedral network formers like water have a special position. Their vast amount of anomalies make the transfer of models like density scaling difficult. We thus use molecular dynamics simulations to examine a family of water-like models produced by systematically varying the partial charges of the SPC/E and TIP4P2005 water models [1]. The geometry of the molecules remains unchanged but the inter-molecular interactions of the models vary strongly. We show that the resulting dynamics spread over a wide temperature range with the glass transition temperature T_g and the high temperature activation energy E_∞ both changing by a factor of five. Models of the glass transition are tested using observables from these studies on water-like models in the bulk and from concomitant work on these systems in confinement which allows us to determine structural and dynamical length scales. Common behavior of the models can be found using a recently proposed empirical function that splits the activation free energy into a constant value E_∞ and an exponentially growing contribution $E_c(T)$ [2]. A common ratio of E_∞/T_g is found. Modification of the partial charges also changes the phase diagram preparing the ground for studies of water's two supercooled phases.
[1] Horstmann, R., and M. Vogel. J Chem Phys **147**, 034505 (2017)
[2] Schmidtke, B. et al., Phys. Rev. E **86**, 041507 (2012)

DY 82.6 Fri 11:15 BH-N 334

Secondary Relaxation Dynamics Observed by Photon-Correlation-Spectroscopy — •Till Böhmer, Jan Gabriel, Andreas Helbling, Florian Pabst, and Thomas Blochowicz — TU Darmstadt, Institut für Festkörperphysik, Germany

Secondary relaxation processes in simple molecular glass formers have been a long-standing topic in research of supercooled liquids and amorphous solids. In particular understanding the mechanism behind Johari-Goldstein-β-relaxation is considered to be important, because it originates from the dynamic of the entire molecule and is expected to be a universal feature of the glass-transition.

To obtain a new perspective, photon-correlation-spectroscopy (PCS) was utilized to examine reorientational dynamics in various monohydroxy alcohols. After improvements regarding the experimental setup secondary relaxation processes were successfully resolved in PCS. By comparing the results of light scattering experiments with those of broadband dielectric spectroscopy, focusing on the differences in amplitude and shape of the respective processes, insight on the mechanism behind the JG-β-relaxation can be gained.

15 min. break

DY 82.7 Fri 11:45 BH-N 334

Emergent Many-body Interactions and Inapplicability of Hard Sphere Jamming Theory — •Yoav G. Pollack[1], Murari Singh[1], Giorgio Parisi[2], Corrado Rainone[1], and Itamar Procaccia[1] — [1]Weizmann Institute of Science, Israel — [2]Sapienza Universit di Roma, Italy

The mechanism of jamming in soft matter was recently argued to be dimensionally independent by studying the scaling exponents predicted

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within an infinite-Dimensional mean-field hard-sphere theory. The predicted critical exponents were found to match surprisingly well the numerical measurements in finite-D including 2D and 3D. Such a match seemingly suggests that the infinite-D theory is applicable to realistic systems. Our current work addresses the puzzle of this lack of strong D dependence usually observed in critical phenomena.

We study the jamming transition using *effective* inter-particle forces. In thermal materials where nevertheless the mean positions are well defined on a given time-scale, these effective forces are what keeps the particles "in place". We observe emergent effective many-body forces, and quantify the non-binary contributions Vs. proximity to jamming. For hard spheres the effective forces are binary *precisely* at jamming, similarly to the infinite-D limit and propose that this explains the match of theory and measurements. We further conclude that the predictions of infinite-D hard spheres should not be inapplicable to more realistic particles which are never absolutely hard[1].

[1]G. Parisi, Y.G. Pollack, I. Procaccia, C. Rainone and M. Singh, Submitted for publication, arXiv:1709.01607.

DY 82.8 Fri 12:00 BH-N 334

Controlled crystallization of luminescent lithium borate glasses — •A. Charlotte Rimbach[1], Juliane Schuppich[1], Bernd Ahrens[1,2], Franziska Steudel[2], and Stefan Schweizer[1,2] — [1]South Westphalia University of Applied Sciences, Lübecker Ring 2, 59494 Soest — [2]Fraunhofer Application Center for Inorganic Phosphors, Branch Lab of Fraunhofer Institute for Microstructure of Materials and Systems IMWS, Lübecker Ring 2, 59494 Soest

Lanthanide-doped borate glasses are promising candidates as frequency-converter for LED applications. The borate glass system provides high transparency in the visible spectral range, good lanthanide ion solubility and high mechanical stability. The lanthanide ions terbium (Tb^{3+}) and europium (Eu^{3+}) show a bright luminescence therein with quantum efficiency values of approx. 60 % (486 nm excitation) and 90 % (396 nm excitation), respectively. However, since the absorption coefficient of the lanthanide ions is low, only a small amount of the excitation light is absorbed resulting in a poor conversion efficiency. To increase the optical absorption by prolonging the optical pathway through multiple scattering within the glass, the as-made luminescent borate glasses are processed to glass ceramics. The focus of this work is on the analysis of the crystallization process by means of differential scanning calorimetry (DSC), in situ x-ray diffraction (XRD) as well as optical spectroscopy and quantum efficiency (QE) measurements.

DY 82.9 Fri 12:15 BH-N 334

Glassy dynamics as reflected in its inter- and intra-molecular interactions — •Friedrich Kremer, Wilhelm Kossack, and Markus Anton — Institute of Experimental Physics I, University of Leipzig, Linnéstr. 5, 04103 Leipzig, Germany

The inter- and intra-molecular interactions of low molecular weight and polymeric glass-forming model systems are studied by Broadband Dielectric (BDS) - and Fourier-Transform Infrared (FTIR) - Spectroscopy. Analyzing the temperature dependencies of specific IR absorption bands, reflecting the intramolecular potentials of dedicated molecular moieties, enables one to unravel on an intramolecular scale the process of glass formation and to compare it with the dielectrically determined primarily intermolecular dynamics. Molecular systems to be studied are typical glassformers as glycerol, propyleneglycol, poly-propyleneglycol, propylenecarbonate and polypropylencarbonate. By that a wealth of novel information is obtained proving that the different molecular moieties of a glass former show often strongly different characteristic, temperature dependencies. This demonstrates the fundamental importance of intra-molecular dynamics giving refined insights into the underlying interactions beyond coarse-grained models treating the glassformer as rigid body.

DY 82.10 Fri 12:30 BH-N 334

Site energy distributions in ion conducting glasses — •Martin Schäfer and Karl-Michael Weitzel — Philipps-Universität Marburg, Marburg, Germany

In a crystalline sample of an ion-conducting material all ions exhibit the same surrounding and thus the same site energy. In an ion-conducting glass ions exhibit different local surroundings. Thus, a distribution of site energies will apply. So far all information on such site energy distributions appears to either come from theory or indirect experiments. This site energy distribution is evidently crucial for all transport processes involving the transport of considerable fractions of mobile ions, e.g. in battery materials. Consequently, direct information on this energy distribution best comes from an experiment, where all ions of a certain kind are almost completely depleted, e.g. by a foreign ion. By reanalysis of previously published concentration depletion profiles within the foreign ion bombardment induced ion transport [1] we are now able to derive the complete site energy distribution of sodium ions in a calcium-sodium-phosphate glass. The occupied part of the site energy distribution spans a width of about 0.28 eV FWHM [2].

[1]*L. Rossrucker, P.V. Menezes, J. Zakel, M. Schäfer, B. Roling and K.-M. Weitzel, Zeitschrift für Physikalische Chemie, 226, 341-353, (2012).
[2]*M. Schäfer, K.-M. Weitzel, to be submitted