

DY 10: Glasses and Glass Transition (joint session CPP/DY)

Time: Monday 16:15–17:30

Location: H8

DY 10.1 Mon 16:15 H8

A coarse-grained model for studying polymer melts toward the glass transition point under cooling — ●HSIAO-PING HSU and KURT KREMER — Max Planck Institute for Polymer Research, Mainz, Germany

For studying polymer melts of weakly semiflexible chains under cooling at zero pressure by molecular dynamics simulations, a coarse-grained model based on the standard bead-spring model is developed. We introduce a short range attractive potential between non-bonded monomers such that the pressure of polymer melts is tuned to zero. Additionally, the common used bond-bending potential [Everaers et al., *Science* 303, 823 (2004)] controlling the chain stiffness is replaced by another new bond-bending potential. With our newly developed model, we show that the Kuhn length and the internal distance of chains in a melt are independent of temperatures under cooling. The glass transition is probed by the volume change of polymer melts and the slowing down of the mobility of chains. Thus, our coarse-grained model can be served as an optimal model for studying glass-forming polymer melts and understanding the effect of free surface on the glass transition of thin polymer films.

DY 10.2 Mon 16:30 H8

Molecular Dynamics of Dipole Functionalized Triphenylene-based Discotics — ●ARDA YILDIRIM¹, ANDREA BÜHLMAYER², SHUNSUKE HAYASHI³, JOHANNES CHRISTIAN HAENLE², KATHRIN SENTKER⁴, PATRICK HUBER⁴, SABINE LASCHAT², and ANDREAS SCHÖNHALS¹ — ¹Bundesanstalt für Materialforschung und -prüfung (BAM), Unter den Eichen 87, 12205 Berlin, Germany — ²Institut für Organische Chemie, Universität Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany — ³Department of Applied Chemistry, Ritsumeikan University, Kusatsu, Shiga 525-8577, Japan — ⁴Materials Physics and Technology, Hamburg University of Technology (TUHH), 21073 Hamburg, Germany

In this study, the molecular dynamics of a series of dipole functionalized triphenylene-based discotics, forming a columnar mesophase, were investigated by broadband dielectric spectroscopy (BDS). In addition to conductivity and localized dynamics, glassy dynamics were also observed. At higher temperatures an α_1 -processes and at low temperatures an α_2 processes were detected having a completely different temperature dependence of its relaxation times. Different molecular assignments of α_1 - and α_2 -processes are suggested. The phase behavior of the material was explored under helium purge down to 100 K by differential scanning calorimetry (DSC). Besides the phase transition temperatures and enthalpies, one or two thermal glass transitions were found for all the materials. Moreover, the glassy dynamics were further investigated by Flash DSC, which is a chip-based calorimetry technique allowing for fast heating and cooling rates as high as 10000K

DY 10.3 Mon 16:45 H8

System size-dependent non-affine displacements in a model glass: the impact of yield strain — ●MOUMITA MAITI and ANDREAS HEUER — University of Muenster, Institute for physical chemistry, Corrensstr. 28/30, 48149, Muenster

The probability distribution of non-affine displacements has an exponential tail, which is scaled with the system size. The scaling exponent is zero for all strains below a critical value which turns out surprisingly to be the overshoot strain. Above, the scaling exponent is finite. This picture holds for the system size larger than approx. 4000 particles. For small system size we find that the scaling exponent is finite and

constant irrespective of any strain value. In order to understand these two pictures we calculate the mobility correlation of nearest neighbours. Around the mobility range where percolation of mobile particles takes place, the correlation increases again up to sizes of approx. 4000 particles and saturates above that size. This yields additional insight into the physical mechanisms of yielding.

DY 10.4 Mon 17:00 H8

Tuning the Temperature-Dependent Thermal Conductivity via Complex Colloidal Superstructures — FABIAN NUTZ and ●MARKUS RETSCH — Physical Chemistry I, University of Bayreuth, 95447 Bayreuth, Germany

The ability to specifically tune the temperature dependence of the thermal conductivity possess a vital challenge to develop and conceive future heat management devices. In this contribution, we demonstrate the vast potential of polymer colloidal crystals to address and master these challenges. We achieve this goal based on the constriction controlled thermal transport through well-defined colloidal crystal superstructures.[1,2,3,4] These colloidal superstructures are specifically built by tailor-made latex particles with distinct glass transition temperatures. We exploit their multiresponsive film formation at various temperatures to demonstrate unprecedented control over thermal conductivity at temperatures between 25 °C and 200 °C. Based on the film formation process, we can irreversibly increase the thermal conductivity by a factor of about three. We show how to control: i) the temperature, where the increase in thermal conductivity happens ii) the sharpness of the thermal conductivity increase iii) the height of the increase in thermal conductivity iv) the incorporation of a multistep increase in thermal conductivity

[1] Nutz et al. *J. Colloid Interface Sci.* 2015, 457, 96. [2] Ruckdeschel et al, *Nanoscale* 2015, 7, 10059. [3] Nutz et al, *Phys. Chem. Chem. Phys.* 2017, 19, 16124

DY 10.5 Mon 17:15 H8

Direct Determination of the Thermodynamic Properties of Melting for Amino Acids — ●Y.Z. CHUA¹, H.T. DO³, D. ZAITSAU², S.P. VEREVKIN², C. HELD³, and C. SCHICK¹ — ¹Uni. Rostock, Inst. Physics and CALOR, Rostock, Germany — ²Uni. Rostock, Inst. Chemistry, Rostock, Germany — ³TU Dortmund Uni., Depart. Biochem. Chem. Eng., Dortmund, Germany

The properties of melting are used for the prediction of solubility of solid compounds. Unfortunately, by using the conventional DSC or adiabatic calorimetry direct determination of the melting enthalpy and melting temperature is often not possible for biological compounds due to the decomposition during the measurement. The apparent activation energy of decomposition is at least one order of magnitude smaller than that of melting. This allows shifting of the decomposition process to higher temperature without seriously disturbing the melting by applying very high heating rates. High scanning rates up to $2 \cdot 10^4 \text{ K} \cdot \text{s}^{-1}$ are utilized with fast-scanning calorimeter Mettler Toledo Flash DSC1, which employs thin film chip sensors with sub $\mu\text{J} \cdot \text{K}^{-1}$ addenda heat capacities. With the help of this technique the melting parameters for a series of amino acids and dipeptides were successfully determined. The ultra-fast cooling of the melted samples allows the studied compounds to retain in the liquid state and to determine for the first time its glass transition temperatures. The determined glass transition temperatures agree with the Beaman-Kauzmann rule. The correlation between the melting properties of the amino acids and dipeptides with their molecular structures were investigated.