CPP 37: Nanostructures, Nanostructuring and Nanosized Soft Matter

Time: Wednesday 15:00–16:15 Location: MER 02

CPP 37.1 Wed 15:00 MER 02

Structure and dynamics of a 1,4-polybutadiene melt in an alumina nanopore: A molecular dynamics study — •Lama Tannoury[1], Mathieu Solar[2], and Wolfgang Paul[1] — [1]Martin-Luther-Universität Halle-Wittenberg — [2]Université de Strasbourg

The study of the structure and dynamics of polymer melts confined by solid surfaces enhances our knowledge about the glass transition temperature as well as that of composite materials. It has been shown that conformations and dynamics of polymer melts confined to thin films and flat surfaces as well as cylindrical pores are altered in comparison with the bulk. The change in properties depends on several factors including but not limited to the geometry of confinement. In this research, we study the effects of both nanoscopic confinement and curvature on the dynamics and properties of a chemically realistic 1,4-polybutadiene (PBD) melt using Molecular Dynamics (MD) simulations. We investigate the density layering across the nanopore as well as the orientational ordering in the melt on both the segmental and chain scales. As for the dynamics, we show that the confinement creates an adsorbed layer that not only slows down the relaxation but also creates a third step not present in the bulk. The system has also been investigated by different experimental techniques, allowing for a comparison of our simulations to the experimental data.

CPP 37.2 Wed 15:15 MER 02

Toluene-mediated morphology transition of amphiphilic diblock copolymer templated Si/Ge/C thin films — •Christian L. Weindl[1], Kexin Wu[1], Christian E. Fajman[2], Constantin Harder[3], Benedikt Sochor[3], Matthias Schwartzkopf[3], Stephan V. Roth[3,4], Thomas F. Fässler[2], and Peter Müller-Buschbaum[1,5] — [1]TUM School of Natural Sciences, Chair of Functional Materials, 85748 Garching — [2]TUM School of Natural Sciences, Chair of Inorganic Chemistry with Focus on Novel Materials, 85748 Garching — [3]DESY, 22607 Hamburg — [4]Royal Institute of Technology KTH, 100 44 Stockholm — [5]MLZ, TUM, 85748 Garching

The latest research has revealed promising results for silicon (Si) and germanium (Ge) as anode materials for lithium-ion batteries. These two group 14 semiconductors are considered auspicious additives in graphite anodes due to their high specific capacity (Si) and electron mobility (Ge). This study aims to synthesize a mesoporous Si/Ge/C structure over a wet chemical sol-gel approach with the structure-directing amphiphilic diblock copolymer PS-b-PEO and the Zintl cluster $K_{12}Si_xGe_{17-x}$. Furthermore, we added toluene as an additive to further induce the microphase separation. Real-space data as SEM will be discussed with the reciprocal-space analysis methods as grazing-incidence small/wide-angle x-ray scattering (GISAXS/GIWAXS). Finally, as an application, we will show the performance of these novel films as Li-ion battery anodes.

CPP 37.3 Wed 15:30 MER 02

Ultracompact Beam Deflector using Electrically Switchable Metallic Polymer Nanogratings — •Yohan Lee, Julian Karst, Monika Ubl, Mario Hentschel, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569, Stuttgart, Germany

We introduce nanogratings from metallic polymers which show an electrochemically-driven optical metal-to-insulator transition. A key feature of the design is separately addressable electrodes to vary the superlattice period of the grating via the applied voltages. Thus, the proposed ultracompact beam deflectors can generate various angles.

CPP 37.4 Wed 15:45 MER 02

Molecular dynamics of superglassy polymers for gas separation by neutron scattering, dielectric spectroscopy, and calorimetry — •Paulina Szymoniak[1], Mohamed Aejaz Kolmangadi[1], Reiner Zorn[2], and Andreas Schönhals[1] — [1]Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany — [2]Forschungszentrum Jülich, Jülich Centre for Neutron Science, Jülich, Germany

Janus polytricyclononenes (PTCN) with rigid backbones and flexible n-alkyl (n=propyl-decyl) are innovative materials that show potential in separating hydrocarbons. These superglassy polymers were designed to show an enhanced, controllable gas permeability via flexible alkyl side chains. PTCNs show nanophase separation between the alkyl side chains and the backbones with a distinct α-relaxation of the alkyl-rich nanophase found by broadband dielectric spectroscopy and temperature modulated DSC. Further, Janus PTCNs were studied by quasielastic neutron scattering (QENS) employing backscattering and time of flight instruments. For an overview of dynamic processes inelastic fixed window scans were performed showing segmental motions of alkyl-rich nanodomains and an additional low temperature relaxation, assigned to methyl group rotations. The molecular mobility was extracted from a combined analysis of backscattering and time of flight QENS data. The glass transition of the backbone-rich domains, which is beyond or near to the degradation of the materials, was evidenced by fast scanning calorimetry by decoupling it from decomposition, employing high heating rates.

CPP 37.5 Wed 16:00 MER 02

Size matters: Size Effects on Surface Chemistry and Raman Spectra of Sub-5 nm Oxidized High-Pressure High-Temperature and Detonation Nanodiamonds — •Bernhard Schummer[1] and Stepan Stehlik[2] — [1]Fraunhofer Development Center X-ray Technology, 90768 F*urth, Germany — [2]Institute of Physics of the Czech Academy of Sciences, 162 00 Prague 6, Czechia

Materials with very small dimensions of a few nanometers is of major importance for fundamental science as well as innovative applications. Those nanomaterials show different effects like quantum size effects, structural transformation or phonon-confinement effects. It has been predicted theoretically that nanodiamonds (NDs) have a structural transformation and phonon-confinement effect below 3 nm in size. Here, we investigate how size effects the surface chemistry, microscopic structure, and Raman scattering of high-pressure high-temperature (HPHT) and detonation nanodiamonds (DNDs) between 2 to 3 nm. The particle size and particle size distribution (PSD) of those different fractions was analyzed with dynamic light scattering, analytical ultracentrifugation, small-angle X-ray scattering, X-ray diffraction, and transmission electron microscopy as complementary techniques. Comprehensive comparison of detonation and pure monocrystalline HPHT NDs reveals effects of diamond core size and defects, chemical and temperature (in)stability, and limitations of current phonon confinement models.