

CPP 6: Composites and Functional Polymer Hybrids I

Time: Monday 11:30–13:00

Location: H 0106

Invited Talk

CPP 6.1 Mon 11:30 H 0106

Stretchable, redispersible, recyclable: reversible interfaces for electrically conductive hybrids and composites — ●TOBIAS KRAUS — INM - Leibniz-Institute for New Materials, Saarbrücken, Germany — Saarland University, Colloid and Interface Chemistry, Saarbrücken, Germany

Composites and hybrids with organic polymer and inorganic particle components are indispensable for modern products. This talk focuses on electrically conductive hybrids and composites. We study their structure and internal interfaces to make them reversibly stretchable, enable repair, and simplify their recycling. Reversible interfaces provide functional connections that can be released with a stimulus, for example when components must be separated at the end of product lifetime. I will first discuss fundamental results on the redispersion of agglomerated particles at different length scales. Particle deagglomeration in water and non-polar organic solvents is introduced. Reversibility at the nanometer scale is then discussed for the case of printed electronics. Inks based on hybrid particles with metal cores and ultrathin layers of conductive polymers were developed as sinter-free, inkjet-printable conductors. I will show that the particles can be re-dispersed and recovered to create new inks at the end of product lifetime. As an outlook, I will discuss the role of reversible interfaces in stretchable electronics. The 3D reconstruction of conductive networks using Focused Ion Beam-Scanning Electron Microscopy tomography and leads to first results on structure-property relations for piezoresistance and ageing after many cycles.

CPP 6.2 Mon 12:00 H 0106

Effects of the particle packing structure on the thermal conductivity of filled polymer composites — ●OLIVER ROSER^{1,2}, ANDREAS GRIESINGER³, and OTHMAR MARTI² — ¹Center for Heat Management (ZFW), Stuttgart — ²Institute of Experimental Physics, Ulm University — ³Baden-Wuerttemberg Cooperative State University (DHBW), Stuttgart

For a wide range of applications, polymers are modified with granular fillers to improve thermal conductivity. In addition to the filler concentration and the thermal properties of the polymer and fillers, it is predominantly the microscopic packing structure that affects the composite's achievable thermal conductivity. The attainable microscopic packing structure is dependent upon particle shape, size distribution, and agglomeration behavior, resulting in more or less effective thermal networks. For a detailed analysis of these effects, we have developed a new microscale modeling approach in which the filler packings are represented in geometric detail. Experimentally determined size distribution and shape data of the filler particles are used as input and enable the modeling of arbitrary filler materials. In this talk, we describe the new calculation strategy, the findings from the studies that have been performed on the microstructure of the filled polymer composites, and an experimental validation of the new calculation method.

CPP 6.3 Mon 12:15 H 0106

Multi-scale model of the conductivity of diblock copolymer system filled with conductive fillers. — ●ALEXANDER CHERVANYOV — University of Münster, Münster, Germany

We investigate the electrical response of the insulating diblock copolymer system (DBC) filled with conductive fillers depending on the following factors: (i) composite temperature and morphology; (ii) affinities of fillers for copolymer blocks; (iii) interaction between fillers. By performing consistent phase-field and Monte-Carlo simulations of a filled DBC system, we demonstrate that the location of fillers in DBC essentially depends on the above three factors. The simulated dis-

tribution of fillers in DBC, in turn, proves to be directly related to the electrical response of the composite, calculated by the developed model. In particular, the order-disorder transition in DBC system is found to co-occur with the insulator-conductor transition in the filler network provided a sufficient difference between the affinities of fillers for dissimilar DBC blocks. The order-order transition between the lamella and cylindrical morphologies of DBC is found to cause a spike in the composite conductivity.

CPP 6.4 Mon 12:30 H 0106

The sensitive aspects of modelling polymer-ceramic composite solid-state electrolytes by molecular dynamics simulations — ●MELANIA KOZDRA¹, DANIEL BRANDELL¹, CARLOS MOYSES ARAUJO², and AMBER MACE¹ — ¹Uppsala University, Uppsala, Sweden — ²Karlstad University, Karlstad, Sweden

One important category of electrolytes for solid-state lithium batteries are composites of ion conducting ceramic (e.g. LLZO) and polymeric (e.g. PEO) materials. In these, Li-ion transport phenomena at the solid-solid interfaces are crucial. Using molecular dynamics (MD) techniques, we here study an interface composed of LLZO and LiTFSI-doped PEO. Although the aim of combining these materials is to utilize the advantages of each phase, both increasing and decreasing ionic conductivity has been observed as compared to the homogeneous phases. The knowledge gap regarding ionic transport processes can to a large part be attributed to difficulties in studying the ceramic-polymer interface. Here, modelling can provide insights. One of the main challenges to overcome then, however, is to understand how a sufficiently robust atomistic model can be constructed in order to provide reliable results. Therefore, a series of MD simulations are here carried out with a variation of certain structural and pair potential parameters, to test how sensitive the outcome is to each variation. Considering that atomistic studies concerning an interface of these materials are scarce, the work will hopefully spark more in silico activities to enhance the perspectives on Li-ion transport phenomena in these composite materials.

CPP 6.5 Mon 12:45 H 0106

Non-Systematic Ion-Specific Effects in Aqueous Au Nanoparticle (NP) Suspensions and Polymer-NP Composites — ●PHILIPP RITZERT, ALEXANDRA STRIEGL, and REGINE V. KLITZING — Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstr. 8, 64289 Darmstadt, Germany

Nanocomposites based on inorganic gold nanoparticle (AuNP) inclusions inside an organic matrix (e.g. polymer brushes) are employed in various fields: catalysis, material engineering, and medicine. Despite numerous demonstrations of AuNPs agents for medical and environmental applications, real world environments still present challenges due to a wide variety of interfering stimuli, e.g. ionic contaminations. Therefore, characterisation of AuNPs response to environmental stimuli is key for the usage in real world applications. The most prominent stimulus in medical applications is the presence of salts. The human body and similar environments pose many salty problems that AuNPs composite materials often attack indirectly. To characterise the ion-specific response of different AuNPs in various salt solutions we systematically employ absorption spectroscopy, transmission electron microscopy, atomic force microscopy. Our model system relies on AuNPs of two sizes and two cappings. We monitor the ion-specific response of AuNPs in suspension for various sodium salts along the Hofmeister series (anion: F, Cl, Br, I, SCN) over time. The ion-specific response of the suspensions is highly dependent on the specific anion. In addition, we immobilise the AuNPs in a polymer brush and subsequently characterise the structural rearrangement in salt solutions.