

CPP 23: Charged Soft Matter

Time: Tuesday 14:00–15:30

Location: H40

CPP 23.1 Tue 14:00 H40

Ionic conductivity of plastic crystals — •DANIEL REUTER, KORBINIAN GEIRHOS, PETER LUNKENHEIMER, and ALOIS LOIDL — Experimental Physics V, University of Augsburg, Germany

Regarding the challenges of storing solar and wind energy or of electro mobility, the development of new solid-state electrolytes is often seen as a promising way to achieve further advances [1]. However, the development of a solid electrolyte with conductivity comparable to that of liquid electrolytes and mechanical properties of a solid is still in progress. There is a whole class of materials naturally combining properties of liquid and solid matter, namely the plastic crystals (PC). Below a certain transition temperature, the molecules of these materials form a well-defined crystalline lattice but still retain their orientational degrees of freedom. This feature of freely rotating molecules ordered in a crystalline structure is believed to enhance the mobility of dissolved ions in the material [2]. Remarkably, by adding a second component to one of the most prominent ionically conducting PCs, succinonitrile, an increase of the conductivity over several decades was found [3]. Therefore dielectric spectroscopy being sensitive to both molecular motion and ionic conductivity was applied to various molecular compositions of two-component PCs. We aim at answering the question if either the possible "revolving door" mechanism or defects in the lattice structure govern the high ionic charge mobility in these binary PC systems.

[1] J. Motavalli, *Nature* **526**, 96 (2015). [2] P. Alarco *et al.*, *Nature* **3**, 476 (2004). [3] K. Geirhos *et al.*, *J. Chem. Phys.* **143**, 081101 (2015).

Invited Talk

CPP 23.2 Tue 14:15 H40

Challenges and opportunities of nanostructured block copolymer membranes for lithium-ion batteries — •EZZELDIN METWALLI, MAJID RASOOL, SIMON BRUNNER, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

The ionic conductivity in relation to the morphology of lithium-doped high-molecular-weight polystyrene-block-polyethylene oxide PS-*b*-PEO diblock copolymer films was investigated as solid state membranes for lithium ion microbatteries.[1] The tendency of the polyethylene (PEO) block to crystallize is highly suppressed with increasing both the salt doping level and the temperature. The PEO crystallites completely vanish at a salt doing ratio of $\text{Li}/\text{EO} > 0.08$, where the PEO segments are hindered from entering the crystalline unit of PEO chain. The increase of the lamella spacing D of the Li-ion/BC hybrid films with increasing Li salt doping level is attributed to the PEO chain conformation rather than the salt volume contribution or the previously reported increase of the effective interaction parameter. Upon salt upload, the PEO chains change from a compact/highly folded conformation to an amorphous/expanded-like conformation. The ionic conductivity is enhanced by the PEO amorphization. We will further emphasize on the challenges related to the low conductivity of the Li-ion/BC membranes at room temperature which limit their practical implementation. Possible solutions are also suggested. [1] E. Metwalli *et al.*, *ChemPhysChem* **16**, 2882 (2015)

CPP 23.3 Tue 14:45 H40

Influence of DMSO-water solvent mixtures on counterion condensation behavior of lithium ions on sulfone based sulfonic acid based dimers. — •ANAND NARAYANAN KRISHNAMOORTHY, CHRISTIAN HOLM, and JENS SMIATEK — Institute for computational physics - University of Stuttgart

Molecular dynamics simulations were performed to study the solvation behavior of sulfone based sulfonic acid dimers in DMSO(Dimethyl sulfoxide) - water mixtures. Previous study show that the non ideality of the binary mixture solution is due to the cluster formation of DMSO and water molecules through hydrogen bonds between donor DMSO

oxygen atom and hydrogen atom of water. This non-ideal behavior is also observed in ionic condensation behavior of lithium ions on dimer surface for specific mole-fractions of DMSO-water mixtures. It is seen that the activity of DMSO drives the counterion condensation behavior of lithium ion on the dimer surface. The non-ideal behavior, we observe can be related to solvent-solvent interactions and preferential solvation of the dimer and the counter ions. In addition the non-ideal nature of the pure DMSO-water mixture is also seen in the diffusive behavior of the solvents and reduced diffusivity is witnessed in presence of the solute(dimer) and qualitatively support the experimental results.

CPP 23.4 Tue 15:00 H40

Ion Pairing and Charging at Nanodroplet Surfaces in Oil/Water Emulsions — •BJÖRN BRAUNSCHWEIG¹, CHRISTIAN SAUERBECK¹, ANDREAS KRAUSE², FRANK R. BEIERLEIN², TIMOTHY CLARK², and WOLFGANG PEUKERT¹ — ¹Institute of Particle Technology — ²Computer Chemistry Center, FAU Erlangen-Nürnberg

Molecular structures and interactions at oil/water interfaces are of great importance for emulsions and their properties such as stability or rheology. In our contribution, we demonstrate that not only the emulsifier coverage and structure, but also the solvation at the interface can significantly influence adsorption. Interfacial properties of emulsions were studied as function of sodium dodecyl sulfate (Na^+DS^-) and NaCl electrolyte concentrations. Experimental results from second-harmonic light scattering at the surface of nanodroplets with a mean radius of 83 nm were corroborated by extensive molecular dynamics (MD) simulations of hexadecane/water interfaces. We have experimentally determined the maximum surface excess of DS-anions ($2.6 \mu\text{mol}/\text{m}^2$) and the Gibbs free energy of adsorption (ΔG) in the presence of Na^+ . Comparing 0 to 5 mM NaCl concentrations we show that ΔG changes from -34 to -41 kJ/mol. This change in ΔG is attributed to a formation of contact ion pairs (CIPs) between DS^- anions and Na^+ cations, which have a higher propensity to adsorb at the hexadecane/water interfaces. MD simulations clearly show that CIPs are formed and thus strongly corroborate conclusions from our experiments. In fact, MD simulations provide a more complete picture of Na^+ , DS^- and water molecules at and near the interfacial region.

CPP 23.5 Tue 15:15 H40

Binding quantification by photochemically triggered microscale electrophoresis — •FRIEDERIKE M. MÖLLER, MICHAEL KIESS, and DIETER BRAUN — Systems Biophysics, Nanosystems Initiative and Center for NanoScience, LMU Munich, Germany

Intricate feedback situations arise when chemical reactions are coupled to physical transport mechanisms. Self-organized patterns are well known for spatio-temporally controlled reaction-diffusion scenarios mostly in biology, but also in geology and chemistry. Here we use the light triggered dissociation of one reaction to create local electrical fields which enable the measurement of the association strength of another reaction.

In more detail, the photoactive compound *o*-nitrobenzaldehyde (*o*-NBA) dissociates upon UV irradiation and releases a proton. Differential diffusion of the charged photoproducts perturbs electroneutrality and generates a local electrical potential Φ on the low mV scale. Biomolecules move within the electrical field by electrophoresis. Due to backdiffusion on the microscale, concentration profiles settle within seconds proportional to $\exp(-\mu/D\Delta\Phi)$. The diffusive character of transport makes the local, aqueous electrophoresis size selective.

We exploit the size selectivity for the quantification of aptamer-protein affinity in aqueous solution. Using the well characterized thrombin aptamer TBA15 as a proof of principle, we succeed in determining the K_D of binding in the nanomolar regime. Our results are in good agreement with literature and thermophoretic binding assays both with and without *o*-NBA.