# CPP 48: P13: Charged Soft Matter

Time: Wednesday 10:00–13:00 Location: Poster A

CPP 48.1 Wed 10:00 Poster A

**Dynamics of the Hydrogen Bond Network of Water** — •Miriam Jahn and Stephan Gekle — University of Bayreuth, Germany

The special properties of liquid water originate from the presence of hydrogen bonds that link the molecules in a preferably tetrahedral arrangement. An evidence of the resulting real network structure is the occurrence of loops of hydrogen bonds. Six and seven-membered loops appear most frequently. As the binding energy amounts to few $k_BT$ this network is highly transient.

Using molecular dynamics simulations of bulk water we analyze the dynamics of the network. Based on the assumption that every hydrogen bond is subject to the same molecular rearrangement processes, loops are expected to be more fragile the more hydrogen bonds they contain. This tendency proves to be true except for three and four-membered loops which are unexpectedly short-lived. We find that loops of five, six or seven molecules experience some stabilization that leads to a longer lifespan than indicated by the same number of randomly grouped hydrogen bonds.

CPP 48.2 Wed 10:00 Poster A

**Shape and Stability comparison of various Nanocellulose Crystals** — •Uhlig Martin[1], Andreas Fall[2], Gustav Nyström[2], Maren Lehmann[1], Sylvain Prèvost[1], Lars Wargberg[2], and Regine von Klitzing[1] — [1]Department of Chemistry, TU Berlin, Berlin, Germany — [2]Department of Fiber and Polymer Technology, KTH Royal Institute of Technology, Stockholm, Sweden

Nanocellulose Crystals (NCC) extracted from native cellulose are a promising natural material. Due to their high stiffness, high aspect ratio, water solubility and low cost they are interesting for a lot of applications e.g. in nanocomposites. The most used NCC is sulfuric acid hydrolyzed NCC. Modifying the NCC, e.g. by carboxylation or coating with polyethylene glycol amine (PEG-NH2) overcomes the problem of aggregation. This contribution focuses on the characterization of modified NCCs using Small Angle Neutron Scattering (SANS), Dynamic Light Scattering (DLS) and Transmission Electron Spectroscopy (TEM). DLS is used to investigate the increase in stability of modified NCC compared to unmodified one. SANS and TEM are used to investigate the change in shape and structure of modified NCC. Uncoated NCC both with sulfate groups and carboxylic groups were analyzed. Polymer coated NCC were prepared, either by electrostatic adsorption of polyethyleneimine (PEI) or chemically grafting of polyethylene glycol amine (PEG-NH2) to the NCC particles surface. Aqueous NCC dispersions where measured at various NCC and polymer concentrations and different polymer molecular weights. SANS data revealed a tendency of the rods to aggregate into 2D-stacks of several rods.

CPP 48.3 Wed 10:00 Poster A

**Developing simultaneous actuating and self-sensing technique for IPMC** — •parisa bakhtiarpour, othmar marti, and masoud amirkhani — Institute of experimental physics, Ulm university, Germany

Electroactive polymer (EAP) is a class of material, which deforms under electrical stimulation. Ionic polymer metal composite (IPMC) is a type that can function in the both wet and dry mediums. IPMC is a perfluorinated sulfonic ionic polymer membrane sandwiched between two metallic electrodes and containing mobile cations and fixed anion. Application of IPMC as a smart material in soft robotic is an emerging and cutting-edge technology with a great potential to benefit aerospace, medical and automotive industry. However, a smart system requires a self-sensing mechanism, which allows interacting with environment and responding correspondingly. In this poster, we present a new simultaneous actuating and sensing technique, which is based on the resistance properties of IMPC across the sample.

CPP 48.4 Wed 10:00 Poster A

**The effect of miniaturization on the performance of IPMC** — •virendra vikram singh, parisa bakhtiarpour, othmar marti, and masoud amirkhani — Institute of experimental physics, Ulm university, Germany

Ionic Polymer Metal composites (IPMC) are electroactive polymer (EAP) that bends in response to a small applied electric field as a result of the mobility of cations in the polymer network. IPMC is made of an Ionic polymer membrane such as Nafion covered on both sides by metallic layers, to form the electrodes. This type of polymer is light material and needs a low driving voltage so it is an excellent candidate for smart microelectromechanical systems (MEMS). However, using IPMC for smart MEMS is still a cutting-edge technology, and many modifications and improvements must be done for real-world applications. As a first step, one should understand the performance of IPMC in the millimeter and micrometer scale. Generally, IPMC thickness is around 0.2 mm but length and width are several orders of magnitude bigger than the thickness. Here we present results of actuating and sensing ability when the width and thickness of IPMC are in the same order of magnitude.

CPP 48.5 Wed 10:00 Poster A

**The charge storage properties and applications of polymer brush electret** — •Xinlei Ma — Research Center for Bioengineering and Sensing Technology, University of Science & Technology Beijing, Beijing 100083, People's Republic of China.

Electrets are dielectric materials that can store electrostatic charge over a long time scale. Although benefitting from the charge storage, such materials are widely used in electronics, machinery and biological systems. , challenges remain in principles explanation, facial processing and applications. The polyelectrolyte brush, which anchoring to a substrate with one end of the polymer chain and maintaining lots of fixed ions and counter ions on the surface will bring a further scope on the charge storage mechanism of polymer electrets. Of note, the polyelectrolyte brushes exhibit excellent environment robustness and well-organized chain conformation. Those properties endow superior control over surface structures and functionalities such as film morphology, grafting density, chemical composition, and many other surface properties, which will provide a feasible means to complicated structure fabrication and flexible sensor architecture.

CPP 48.6 Wed 10:00 Poster A

**Simulation of ionic solutions with the extended ReaxFF+ force field** — Oliver Böhm, •Stephan Pfadenhauer, and Philipp Plänitz — AQcomputare GmbH, 09125 Chemnitz, Germany

The ReaxFF+ [1] force field is an extension of the original bond order dependend reactive force field (ReaxFF) of the van Duin group [2]. The capability of the ReaxFF+ force field to simulate ionic solutions is demonstrated on the example of hydrolysis of sodium clusters. The large number of parameters were fitted to DFT ab initio data by means of an improved training algorithm. The predictions of the ReaxFF+ simulations are in good agreement with ab inito results. Therefor we have shown that ReaxFF+ is capable of describing covalent as well as ionic bonds.

[1] O. Böhm, et al., J. Am. Chem. Soc. (2015) submitted

[2] A. van Duin, et al., J. Phys. Chem. A, 105, 9396 (2001); J. Phys. Chem. A, 107, 3803 (2003)

CPP 48.7 Wed 10:00 Poster A

**Quasi-elastic neutron scattering study of a room temperature ionic liquid confined in nanoporous carbon** — •Mark Busch[1], Jan Embs[2], Boris Dyatkin[4], Katie Van Aken[4], Alexei Kornyshev[3], Yury Gogotsi[4], and Patrick Huber[1] — [1]Institut für Werkstoffphysik und Werkstofftechnologie, TU Hamburg-Harburg, Hamburg, Deutschland — [2]Laboratory for Neutron Scattering, Paul Scherrer Institut, Villigen, Schweiz — [3]Imperial College, London, UK — [4]Drexel University, Philadelphia, U. S. A.

We present quasi-elastic neutron scattering measurements of the self-diffusion behaviour of the room temperature ionic liquid 1-N-butylpyridinium bis-((trifluoromethyl)sulfonyl)imide which was confined in nanoporous carbon. Thereby the influence of different pore diameters in the nanometre range on the self-diffusion dynamics has been investigated at several temperatures.

CPP 48.8 Wed 10:00 Poster A

**Solvation of model spheres in different ionic liquids** — •Volker Lesch[1], Andreas Heuer[1], Christian Holm[2], and Jens Smiatek[2] — [1]Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster — [2]Institut für Computerphysik, Uni-

versität Stuttgart

Due to their ionic properties ionic liquids are considered to be solvents for the future. Furthermore, their toxic level is low compared with other solvents. However, in the literature only the solvation of cellulose and zinc finger is investigated via molecular dynamics but no general discussion of solvation effects is available.

In this study, we focus on the solvation of charged and uncharged model spheres in 1-ethyl-3-methylimidazolium (emim) with the anions chloride, tetrafluoroborate, acetate and bis(trifluoromethanesulfonyl)imide. Beside the investigation of different anions, we also simulate the model spheres with different $\epsilon$ values. We found a dramatic influence of the anion size on the structuring of the ionic liquid, especially for the charged spheres.