

BP 24: Bioinspired Functional Materials, Biomaterials and Biopolymers (joint session CPP/BP)

Time: Wednesday 15:00–16:30

Location: PC 203

BP 24.1 Wed 15:00 PC 203

Specific Ion Effects of Protein-Coated Au NPs: The Influence of Hydroxide Formation on Charge and Stability —

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When NPs are exposed to the environment, a protein corona is generated around the NPs. This changes the physicochemical properties of the NPs drastically, especially their colloidal stability, which is a key feature for discovering their bioavailability, toxicity and fate in the environment. In this work, the impact of the type of protein corona on the colloidal stability towards different ions was investigated by using three different proteins. Au NPs were coated with bovine serum albumin, beta-lactoglobulin and insulin and tested against different ions. The particles exhibited a highly pronounced and dissimilar optical response towards various heavy metal ions. The response of the Au@Protein NPs towards the different metal ions strongly depends on the protein coating of the NPs, but also on the specific metal ion and the generation of metal hydroxides. We discovered that the generation of metal hydroxides is the determining factor for the dissimilar colloidal stability of Au@Protein NPs and therefore plays an important and up to now neglected role in the interpretation of specific ion effects.

BP 24.2 Wed 15:15 PC 203

Denaturation-Induced Fiber Formation of Fibrinogen Studied by Small Angle Scattering —

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Over the last years, the interest in materials consisting of biomolecules arranged in nanofibers increased. To get a better understanding of how different environmental parameters affect the fiber formation in solution, we studied the ethanol induced fiber formation of human plasma fibrinogen (HPF) by small angle scattering, i.e., (ultra)small angle neutron scattering and light scattering. To this end, we used water/deuterium oxide and ethanol-d₆ contrast matched at the scattering length density of ethanol-d₆ and varied the protein concentration, as well as ethanol concentration. We find the ethanol-to-water ratio to be a dominant driving force for inducing long fiber formation. Data suggest a 1.5:1 water:ethanol ratio as a threshold, where increasing the water ratio prevents long-fiber formation after an hour of incubation. Time series show, that structure on the protein size-level does not change over time, however the growth in fiber length can still be observed hours after ethanol addition.

This research used resources at the High Flux Isotope Reactor and Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.

BP 24.3 Wed 15:30 PC 203

Direct Determination of the Thermodynamic Properties of Melting for Amino Acids —

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The properties of melting are used for the prediction of solubility of solid compounds. By using conventional DSC or adiabatic calorimetry, direct determination of the melting temperature, T_{fus} , and enthalpy of fusion, $\Delta_{\text{fus}}H$, 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 $2 \cdot 10^4$ K·s⁻¹ are utilized with fast-scanning calorimeter Mettler Toledo Flash DSC1. The melting parameters, e.g. T_{fus} and $\Delta_{\text{fus}}H$, for L-threonine and glycine 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, T_g , which agree with the Beaman-Kauzmann rule ($T_g \approx 2/3 \cdot T_{\text{fus}}$). The entropy of fusion shows significant deviation between the two amino acids. For L-threonine, it was close to the Walden's rule, while for glycine, it was twice smaller. The results are in reasonable agreement with the simulated PC-SAFT values.

BP 24.4 Wed 15:45 PC 203

Cellulose-Based Photoresist for Two-Photon Lithography —

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Lithography is a common method for structuring which uses photoresists based on polymers extracted from mineral oil. To conserve resources those polymers could be replaced by sustainable materials like polysaccharides. So far, no polysaccharide based photoresist has been presented. We here present such a resist by using functionalized cellulose which can be photo-crosslinked by a photoinitiator. For this cellulose and initiator are dissolved in acetone. The resist is curable with two-photon absorption (780 nm) in a direct laser writing system (DLW), and via one-photon absorption with a UV lamp (365 nm), in liquid state as well as in dried state, after evaporation of the acetone. Using DLW and a liquid resist a resolution of 1.6 μm with a feature size of 600 nm is achieved. Furthermore, it is possible to fabricate three dimensional structures. The threshold for polymerization with the DLW depends on the amount of initiator and the amount of acetone influences mainly the durability of the resist.

This resist opens up a new class of photoresist based on sustainable materials.

BP 24.5 Wed 16:00 PC 203

Atomic force microscopy (AFM) based method to investigate the transversal viscoelastic properties of paper fibers —

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It is well known that paper fibers are an inhomogeneous and hierarchical material. Resulting structure-property relations on the fiber scale as well as on the paper scale are complicated and not yet fully understood. To gain more insight on how mechanical properties of fibers are related to properties of the paper, our work focusses on the transverse viscoelastic behavior of single pulp fibers. To reach this ambitious goal we implemented an AFM based method.

Probing nanoscale mechanical properties of soft materials with AFM yields information on the performance of the material. Furthermore, precise force control in AFM methods is possible, and with different contact models, the contact between AFM tip and sample surface can be well described. Here, we use the Johnson-Kendall-Roberts model because it includes adhesion. At the continuum scale, simple empiric models combining springs and dash pots are often used to represent the bulk behavior of viscoelastic materials. Here, some of those models are explained and are used to describe local viscoelastic properties on the nanoscale. Results are presented for kraft pulp and compared to those of viscose fibers which are a simpler model system.

BP 24.6 Wed 16:15 PC 203

Self-consistent Hubbard-corrected DFT study of hole-polaron trapping in glucose-based bio-insulators: the Cyclodextrin case. —

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Using CyDs as an archetypal glucose-based bio-insulator, we use a self-consistent linear response DFT+U approach, as implemented in the linear-scaling ONETEP code, to explore hole-polaron relaxation

both in vacuo and in the presence of different acidic, alkaline and ionic environments due to interacting $H(+)$, $OH(-)$, $Na(+)$ and $Cl(-)$ ions. Hole-polaron trapping in isolated CyDs or in CyDs interacting with $H(+)$, $Na(+)$ and $Cl(-)$ ions is computed to be energetically disfavoured. However, hole-polaron trapping at terminal hydroxyl ($-OH$) groups becomes energetically favoured by up to -2 eV in the presence of alkaline conditions as a result of hydroxyl deprotonation by interacting $OH(-)$ ions. Selective hole-polaron trapping at glycosidic (C-O-

C) bridges between glucose monomers is found to be consistently disfavoured regardless of the presence of interacting ions. The computed stability of the CyD-backbone to direct oxidative depolymerisation, favourable hole-trapping at terminal CyDs hydroxyls, and well known CyDs capability of hosting both organic and inorganic contaminants altogether suggest that CyDs may be effective redox intermediates for the development of novel strategies for photocatalytic oxidation of hosted polluting agents in alkaline conditions.