CPP 35: Poster: Biomaterials and Biopolymers (joint session BP/CPP)

Time: Wednesday 16:30–18:30 Location: Poster C

CPP 35.1 Wed 16:30 Poster C

Structur formation of a coarse-grained bead model — •Benno Werlich[1], Mark Taylor[2], and Wolfgang Paul[1] — [1]Institut für Physik, Martin-Luther University Halle-Wittenberg, Halle(Saale), Germany — [2]Department of Physics, Hiram College, Ohio, USA

We study structure formation of single stiff, coarse-grained hard-sphere chains by means of Wang-Landau type Monte Carlo simulations. Stiffness is introduced by allowing a varying degree of overlap of bonded hard spheres. Collapse of these chains is introduced by a square-well attraction between non-bonded spheres. Depending on the degree of stiffness different, non-trivial morphologies like, e.g., helical structures, occur in the collapsed state. The transitions between different states are determined by an analysis of thermodynamic response functions. For the simulations we implemented the so-called Stochastic Approximation Monte Carlo method which has the advantage of implementing a very general and simple iteration scheme.

CPP 35.2 Wed 16:30 Poster C

Nano-Mechanics of Type I Collagen Fibrils in Aqueous Solution — •Diana Voigt, Julia Hann, Eike-Christian Spitzner, and Robert Magerle — Chemnitz University of Technologie, Institut of Physics, Germany

We investigate purified type I collagen extracted from bovine hide. In aqueous solution, triple helices of collagen molecules (tropocollagens) form fibrils driven by hydrogen bonding processes. Single collagen fibrils, deposited on a silicon substrate, were exposed to an aqueous solution with controlled pH and salt concentration. We use in-situ multi-setpoint intermittent contact mode (MUSIC-Mode) atomic force microscopy for quantitative imaging of collagen fibrils and their mechanical properties in aqueous solution. Furthermore we control the electrochemical potential between the sample and the AFM probe.

CPP 35.3 Wed 16:30 Poster C

Ab-initio molecular dynamics of photoacids in aqueous environment — •Gül Bekcioglu, Christoph Allolio, and Daniel Sebastiani — Institute of Chemistry, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 4, 06120 Halle (Saale)

Biophysical processes often take place based on proton relay along a hydrogen bonded chain.[1] Such proton transfer reactions along "water wires" are difficult to observe directly inside a protein. Photosensitive acid/base systems provide a method to control and study ultrafast proton transport via infrared spectroscopy.[2] Hydroxyquinolines (HQ) are simultaneously photoacids and photobases. Departing from our successful simulation of the excited state dynamics and fluorescence shift of the related N-methyl-6-quinolone [3], we study the ground and excited state solvation of different HQs, focussing on the identification of water wires and excited state protonation dynamics.

[1] H. Luecke, H.-T. Richter, J. K. Lanyi, Science **280** (1998), 1934.
[2] O. F. Mohammed, D. Pines, J. Dreyer, E. Pines and E. T. J. Nibbering., Science **310** (2005), 5745.
[3] C. Allolio, M. Sajadi, N. P. Ernsting and D. Sebastiani, Angew. Chem. Int. Ed. accepted, (2012).

CPP 35.4 Wed 16:30 Poster C

Water absorption of cellulose fibers and possible morphological influences — •Patrice Kreiml[1,2], Christian Ganser[1,2], Roland Morak[1], Oskar Paris[1], Robert Schennach[2,3], and Christian Teichert[1,2] — [1]Institute of Physics, Montanuniversität Leoben, Franz Josef - Str. 18, 8700 Leoben, Austria — [2]Christian Doppler Laboratory for Surface Chemical and Physical Fundamentals of Paper Strength, Graz University of Technology, Petersgasse 16/2, 8010 Graz, Austria — [3]Institute of Solid State Physics, Graz University of Technology, Petersgasse 16/2, 8010 Graz, Austria

Fibers are used in textiles, hygiene products, and medical applications. The water absorption is an important property in the applications mentioned. In this study, the water absorption of different fiber types was measured. The method of choice is a micro balance, which allows to detect a change in mass by increasing and decreasing the partial water vapor pressure at a constant temperature. The result is an isothermal hysteresis that yields the water absorption and desorption with respect to the relative humidity. Additionally, the morphology of two sets of viscose fibers was characterized by atomic-force microscopy (AFM). The two sets of samples were produced under the same conditions, but exhibited a difference in water absorption. A comprehensive roughness analysis showed no significant differences in the roughness parameters. However, on the surfaces of all samples trenches could be observed. Preliminary results indicate an influence of trench density on the water absorption. Supported by Kelheim Fibres and the Christian Doppler Research Society, Vienna Austria.

CPP 35.5 Wed 16:30 Poster C

Hierarchical Multi-Step Folding of Polymer Bilayers — •Georgi Stoychev[1,2], Sebastian Turcaud[3], John Dunlop[3], and Leonid Ionov[1] — [1]Leibniz Institute of Polymer Research Dresden, Hohestr. 6, 01069, Dresden, Germany — [2]Technische Universität Dresden, Physical Chemistry of Polymer Materials, 01062, Dresden, Germany — [3]Am Mühlenberg 1, 14424, Potsdam, Germany

We investigated the actuation of patterned bilayers placed on a substrate. We found that films display several kinds of actuation behavior such as wrinkling, bending and folding that result in a variety of shapes. Based on experiments and modeling, we argued that rectangular bilayers start to roll from the corners due to quicker diffusion of water. Rolling from long-side starts later and dominates at high aspect ratio[1].

It was also demonstrated that one can introduce hinges into the folded structure by proper design of the bilayers external shape without having to use site selective deposition of active polymers. Experimental observations lead us to derive four empirical rules backed up by theoretical understanding as well as simulations. We then demonstrated how those rules can be used to direct the folding of edge-activated polymer bilayers through a concrete example - the design of a 3D pyramid[2].

[1] Stoychev et al, "Hierarchical Multi-Step Folding of Polymer Bilayers", Adv.Func.Mat., published online Nov 26, 2012

[2] Stoychev et al, "Shape-Programmed Folding of Stimuli-Responsive Polymer Bilayers", ACS Nano, 2012, 6(5), 3925-3934