CPP 44: Poster: Biomaterials and Biopolymers

Time: Wednesday 18:15–21:00 Location: Poster B2

CPP 44.1 Wed 18:15 Poster B2

Macromolecular HPMA-Based drug delivery system - behavior in protein environment — •Xiaohan Zhang[1], Bart-Jan Niebuur[1], Petr Chytil[2], Tomas Etrych[2], Sergey K. Filippov[2], Alexey Kikhney[3], Florian Wieland[3], Dmitri I. Svergun[3], and Christine M. Papadakis[1] — [1]Technische Universität München, Physik-Department, Fachgebiet Physik weicher Materie, Garching, Germany — [2]Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Prague, Czech Republic — [3]European Molecular Biology Laboratory, DESY, Hamburg, Germany

Polymer drug carriers based on N-(2-Hydroxypropyl)methacrylamide (HPMA) copolymers bearing cholesterol moieties have been studied extensively over the past few years, to understand the aggregation behavior and shape of the copolymers in dilute aqueous solutions [1,2]. Above certain concentration, micelle-like nanoparticles (NPs) having ellipsoidal shape are observed. However, there is a lack of knowledge on the behavior of these drug carriers in human blood environment.

We use fluorescence life-time correlation spectroscopy (FLCS) and small angle X-ray scattering (SAXS) to investigate HPMA copolymers that are dissolved in an aqueous solution of human serum albumin (HSA) to reveal the interaction between the NPs and HSA. The size of the NPs is reduced when HSA is present. We suspect that some of the cholesterol moieties bind to HSA and are removed from the nanoparticles.

[1] S. K. Filippov, et al., Biomacromolecules, 2012, 13, 2594
[2] S. K. Filippov, et al., Biomacromolecules, 2013, 14, 4061

CPP 44.2 Wed 18:15 Poster B2

Fabrication and Analysis of graphene quantum dots synthesized by the Electrolysis of Graphite — •Sonja Allani, Stefan Fasbender, and Thomas Heinzel — Heinrich Heine Universität Düsseldorf

Fluorescent graphene quantum dots (GQDs) are prepared by the electrolysis of graphite rods in aqueous solution of NaOH and subsequent treatment with hydrazine hydrate. The method described by Zhang et al. [1] is modified and the influence of the synthesis parameters on the GQDs fluorescence and size is investigated. In order to sort the GQDs by size, dialysis with different membrane pore sizes is realized. Dialysis is also used to obtain a pure GQD solution of pH = 7, providing the opportunity for future use in bioimaging applications. Fluorescence and absorbance spectra are taken and Atomic Force Microscopy is used to determine the GQDs size and shape.

[1] Zhang et al., J. Mater. Chem., 2012, 22, 7461-7467

CPP 44.3 Wed 18:15 Poster B2

Ab initio molecular dynamics simulations of intramolecular hydrogen bonds in low molecular weight polyethylene glycol — •Mariana Kozlowska and Pawel Rodziewicz — University of Bialystok, Ciolkowskiego Str. 1K, 15-245 Bialystok, Poland

Polyethylene glycol (PEG) is an amphiphilic polyol with a wide range of applications in medical, chemical and biological areas. Its structural properties were previously investigated theoretically utilizing classical molecular dynamics simulations. Such studies, however, have not taken the possibility of the formation of intramolecular hydrogen bonds into consideration.

In this work, we use static DFT calculations to analyze in detail intramolecular hydrogen bonds formed in the low molecular weight PEG with two to five repeat subunits. Both red- (O-H...O) and blue-shifting (C-H...O) H-bonds, which control the structural flexibility of PEG, are analyzed. The existence and the strength of intramolecular H-bonds is analyzed utilizing the Quantum Theory of Atoms in Molecule. Car-Parrinello molecular dynamics simulations are used to mimic the structural rearrangements and the H-bond breaking/formation in the PEG molecule at 300 K.

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CPP 44.4 Wed 18:15 Poster B2

Fluorescence properties of Graphene Quantum Dots and Graphene Oxide derived by the thermolysis of citric acid — •Christian Wimmenauer, Stefan Fasbender, and Thomas Heinzel — Heinrich Heine Universität Düsseldorf

Fluorescent graphene quantum dots (GQDs) and graphene oxide (GO) are prepared by thermal decomposition of citric acid. The influence of different heating temperatures and different durations of the thermolysis on the fluorescence properties of GQDs and GO are investigated and a sharp distinction in the absorbance spectra of GQDs and GO is observed. Atomic Force Microscopy is used to determine the GQDs size and shape and the GQDs are sorted by size using dialysis membranes with different membrane pore sizes. Dialysis in deionized water is realized to obtain a pure aqueous GQD solution of pH = 7, allowing the possible use in bioimaging applications.

CPP 44.5 Wed 18:15 Poster B2

Three-dimensional microstructures on flexible substrates fabricated by two-photon polymerization for use as cell substrates and for wetting experiments — •Cristina Plamadeala[1], Johannes Heitz[1], Jaroslaw Jacak[1], Gerda Buchberger[2], Werner Baumgartner[2], Birte Magnus[3], and Rainer Marksteiner[3] — [1]Institute of Applied Physics, Johannes Kepler University Linz, Austria — [2]Innovacell Biotechnologie AG, Innsbruck, Austria — [3]Institute of Biomedical Mechatronics, Johannes Kepler University Linz, Austria

Polymer microstructures with various geometries are written onto a flexible substrate by the technique of two-photon polymerization by a Ti-sapphire femtosecond-laser, which is focused into a liquid acrylate based resin containing a photo-initiator. The microstructures are employed either as three-dimensional tissue scaffold onto which adherent cells can be seeded or are used as topological substrates for wetting experiments. Due to confinement to the microstructures and/or mechanical interaction with the scaffold, the cells are stimulated to grow three-dimensionally and to produce calcium binding proteins. There are some similarities in the way the microstructures are filled by cells and by water in wetting tests. Beyond the use of cell scaffolds, the structures may therefore have other potential applications in the field of microfluidics due to their good wettability and water sustainment.

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Raman spectroscopic investigation of tannin-furanic rigid foams — Andreas Reyer[1], Gianluca Tondi[2], Raphael Berger[1], Alexander Petutschnigg[2], and •Maurizio Musso[1] — [1]Fachbereich Chemie und Physik der Materialien, Universität Salzburg, Hellbrunnerstrasse 34, 5020 Salzburg, Österreich — [2]Fachhochschule Salzburg Campus Kuchl, Markt 136a, 5431 Kuchl, Österreich

Tannin-furanic rigid foams are innovative polymeric materials made of inexpensive organic ingredients, and are usually produced via an acid catalyzed polycondensation reaction between furfuryl alcohol and condensed flavonoids (e.g. Mimosa tannin). These bio-friendly foams have already been proposed e.g. as insulating material for eco-sustainable buildings (green building technology), their most important physical properties being their low thermal conductivity and their high fire resistance. The target of the present study is the Raman spectroscopic characterization of the tannin-furanic rigid foams in order to compare their spectral signature with that of the precursor materials furfuryl alcohol, polymerized furfuryl alcohol, and Mimosa tannin, by means of multi-wavelength Raman spectroscopy (at 1064 nm, 532 nm, and 455 nm laser excitation), thereby including a comparison with infrared spectra reported in recent literature, and a discussion on similarities and differences to the spectral signatures of polymer-like sp2 carbon-based materials, and on the the still preserved organic nature of the tannin-furanic foam.

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rubber elasticity for percolation network consisting of gaussian chains — •kengo nishi[1], mitsuhiro shibayama[2], and takamasa sakai[2] — [1]Georg-August-Universität Göttingen, Göttingen,Germany — [2]The University of Tokyo, Tokyo, Japan

A theory describing the elastic modulus for percolation networks of Gaussian chains on general lattices such as square and cubic lattices is proposed and its validity is examined with simulation and mechanical experiments on well-defined polymer networks. The theory was developed by generalizing the effective medium approximation (EMA)

for Hookian spring network to Gaussian chain networks. From EMA theory, we found that the ratio of the elastic modulus at p, G to that at p = 1, G0, must be equal to G/G0= (p-2/ f)/(1-2/ f) if the position of sites can be determined so as to meet the force balance, where p is the degree of cross-linking reaction. However, the EMA prediction cannot be applicable near its percolation threshold because EMA is a mean field theory. Thus, we combine real-space renormalization and EMA and propose a theory called real-space renormalized EMA, i.e., REMA. The elastic modulus predicted by REMA is in excellent agreement with the results of simulations and experiments of near-ideal diamond lattice gels.

CPP 44.8 Wed 18:15 Poster B2

Tethered Polymers In Shear — •Richard Schwarzl and Roland Netz — Freie Universitaet Berlin, Fachbereich Physik, 14195 Berlin, Germany

We employ Brownian dynamics simulation including hydrodynamic interactions to model the dynamic properties of a polymer under shear flow conditions near a no-slip boundary. Our motivation is the von Willebrand factor, a large glycoprotein in blood. It is a crucial component in regulation of hemostasis. The conformational state of the large multimer determines vWFs ability to bind to other biological components such as collagen or bloodplatelets. Our focus is to build a bridge between single molecule pulling experiments and unfolding of vWF under shear.

CPP 44.9 Wed 18:15 Poster B2

Influence of Spacer Length and Flexibility on the Binding Affinity of Divalent Ligands — •Susanne Liese and Roland R. Netz — Freie Universität Berlin, Fachbereich Physik

We present a quantitative model for the binding of divalent ligand-receptor-systems. We study the influence of the ligand spacer length and flexibility on the overall binding affinity and derive general rules for the optimal ligand design. Therefor, we first compare different polymeric models and determine the probability to simultaneously bind to two neighboring receptor binding pockets. In a second step the binding affinity of divalent ligands in terms of the IC50-value is derived. We find that a divalent ligand has the potential to bind more efficient than its monovalent counterpart only, if the monovalent dissociation constant is lower than a critical value. This critical monovalent dissociation constant depends on the ligand-spacer length and flexibility as well as on the size of the receptor. Regarding the optimal ligand-spacer length and flexibility, we find that the average spacer length should be equal or slightly smaller than the distance between the receptor binding pockets and that the end-to-end spacer length fluctuations should be in the same range as the size of a receptor binding pocket.