# CPP 48: The Collapsed State of Polymers: From Physical Concepts to Applications and Biological Systems (joint session with BP)

Time: Thursday 15:00–17:30 Location: ZEU 250

CPP 48.1 Thu 15:00 ZEU 250

**Collapse and self-organization of polymer structures in poor solvent - A Monte Carlo Study** — •Marco Werner[1,2], Christoph Jentzsch[1,2], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]Technische Universität Dresden, Germany

We investigate poor solvent effects in polymer structures such as single polymer globules [1], collapsed polymer brushes as well as self-assembled lipid bilayer membranes [2] by using the bond-fluctuation model with explicit solvent. Focussing on the coil-to-globule transition of single polymer chains we show that even in the case of very poor solvent our coarse grained lattice model avoids freezing effects and preserves dynamic fluctuations at the polymer-solvent interface in contrast to corresponding implicit solvent models. We demonstrate that fluctuations will be necessary for a complete description of the force-extension curve during the unravelling process of a single polymer globule. In particular in the region of coexistence of collapsed and stretched part we observe a fluctuating ensemble of globules along the chain, which smooths the force-extension curve.

[1] C. Jentzsch, M. Werner, und J.-U. Sommer, J. Chem. Phys. 138 (9), 094902 (2013).

[2] J.-U. Sommer, M. Werner, und V. A. Baulin, Europhys. Lett. 98, 18003 (2012).

CPP 48.2 Thu 15:15 ZEU 250

**Melts of unconcatenated and unknotted polymer rings revisited** — •Joachim Wittmer, Hendrik Meyer, and Albert Johner — Institut Charles Sadron & CNRS, 23 Rue du Loess, 67034 Strasbourg CEDEX 2, France

A paradigmatic example for soft matter systems ruled by topological interactions is provided by melts of unconcatenated polymer rings. Recent computational studies suggest that sufficiently long rings become compact which begs the question of whether the irregular surfaces of these compact objects may be characterized by a finite fractal surface dimension $d_s < 3$. We revisit the scaling analysis of the intramolecular structure factor by Halverson et al. [J. Chem. Phys. 134, 204904 (2011)] claiming $d_s \approx 2.8$. Our analysis suggests that this conclusion might be due to an inappropriate application of the Generalized Porod Law. We present then in the second part of our talk a "decorated Gaussian loop model" which does not require a finite fractal surface dimension $d_s < 3$. In this approach the topological interactions between different rings are taken into account by a self-similar and space-filling random tree of polydisperse Gaussian loops ranging from the entanglement length to a skeleton ring of length $N^{2/3}$. Individual rings are predicted to be marginally compact with an average chain size $R^2 \sim N^{2/3}(1 - 1/N^{1/3})$ where all prefactors have been omitted for clarity. Sluggish $1/N^{1/3}$-corrections to the leading power-law behavior are also shown to arise for other experimentally relevant properties.

CPP 48.3 Thu 15:30 ZEU 250

**Fractal globule as an artificial molecular machine** — •Nechaev Sergei — LPTMS (Orsay, France)

The relaxation of an elastic network, constructed by a contact map of a fractal (crumpled) polymer globule is investigated. We found that: i) the slowest mode of the network is separated from the rest of the spectrum by a wide gap, and ii) the network quickly relaxes to a low-dimensional (one-dimensional, in our demonstration) manifold spanned by slowest degrees of freedom with a large basin of attraction, and then slowly approaches the equilibrium not escaping this manifold. By these dynamic properties, the fractal globule elastic network is similar to real biological molecular machines, like myosin. We have demonstrated that unfolding of a fractal globule can be described as a cascade of equilibrium phase transitions in a hierarchical system. Unfolding manifests itself in a sequential loss of stability of hierarchical levels with the temperature change.

CPP 48.4 Thu 15:45 ZEU 250

**Conformation and Structural Changes of Diblock Copolymers with Octopus-Like Micelle Formation under the Influence of Water Vapor** — •Kirsten Dammertz[1], Masoud Amirkhani[1], Christoph Jentzsch[2], Jens-Uwe Sommer[2,3], and Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm Univeristy — [2]Leibniz-Institute of Polymer Research Dresden — [3]Institute of Theoretical Physics, TU-Dresden

External stimuli like vapors, pressure or electric fields can be used to manipulate the polymer configurations of diblock-copolymers. Due to the conformational flexibility of such polymers, AB-diblock copolymers constitute a valuable tool to develop functional nanomaterials and devices.

We study the conformation and structural response of PS-b-PMMA, PS and PMMA adsorbed on mica under water vapor, respectively. At polymer concentrations below the minimum needed for the development of thin films, octopus-like surface micelles are formed. By applying water vapor to a system containing polar PMMA chains, additional mobility can be provided to the polymers. In contrast, PS is less affected since it does not contain a permanent dipole moment. Furthermore, collapse and decollapse effects were observed.

In addition to AFM measurements, we performed BFM Monte Carlo simulations to analyze the formation process of the micellular structures as well as their response to water vapor.

**Invited Talk** CPP 48.5 Thu 16:00 ZEU 250

**Universal aspects of chromosome folding** — •Angelo Rosa — Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste (Italy)

The dynamics of the mm-long chromatin (*i.e*, DNA+histones) fibers in the cell nucleus is subject to strong topological constraints [Sikorav & Jannink (1994)]. In particular, their incomplete equilibration during interphase [Rosa & Everaers (2008)] results in territorial, crumpled globule-like chromosome conformations [Grosberg *et al.* (1993)].

It has been suggested [Rosa & Everaers, *ibid.*; Vettorel *et al.* (2009)], that this incomplete relaxation might underlie a subtle analogy between interphase chromosomes and corresponding solutions of non-concatenated ring polymers. Here, we start from our recent multi-scale computational approach for explicit construction of equilibrated solutions of giant ring polymers [Rosa & Everaers (2013); see talk by R. Everaers] to further explore the physical and biological consequences of this analogy.

We show that not only the territorial confinement [Cremer & Cremer (2001)] but also other characteristic features of chromosome folding such as their conformational statistics [Sachs *et al.* (1995); Lieberman-Aiden *et al.* (2009)] and the loop-on-loop structure of internal contacts [Cook (2010)] arise as a generic consequence of the polymeric nature of chromosomes. Integrated with biological information on intra- and inter-chromosomal interactions, our results pave the way for the systematic modeling of the nuclear structure and dynamics.

**15 min break**

CPP 48.6 Thu 16:45 ZEU 250

**Effects of nucleosome positioning on condenstation of short and long chromatin fibers** — Robert Schöpflin[1], Oliver Müller[1], Christin Weinberg[1], Vladimir B. Teif[2], Karsten Rippe[2], and •Gero Wedemann[1] — [1]CC Bioinformatics, University of Applied Sciences Stralsund, Stralsund, Germany — [2]Deutsches Krebsforschungszentrum & BioQuant, Heidelberg, Germany

In eukaryotes DNA is associated with proteins in a complex structure termed chromatin. The basic packaging unit of chromatin is the nucleosome in which DNA is wrapped around a histone octamer. Experiments indicate that chromatin has different packaging conditions connected to distinct activation states. Experimental evidence showed that packaging and activation states are closely linked to positions of nucleosomes on the DNA which are actively regulated. To improve the understanding of the interplay between nucleosome positions and chromatin structure we applied computer simulations of a coarse-grained chromatin model including fundamental physical properties such as elasticity, electrostatics and nucleosome interactions using a feedback-optimized replica exchange protocol. We calculated the effect of nucleosome positioning on the structure of polynucleosomes of different length scales, up to the size of a gene locus. We compared chromatin models based on synthetic positions with models based on experimen-

tally derived nucleosome positions from cells at different stages of cell differentiation. Simulation results revealed a significant influence of nucleosome positions on the three dimensional structure of chromatin.

CPP 48.7 Thu 17:00 ZEU 250

**Loop models in Magnetic Spin Ice crystals** — •Ludovic Jaubert[1], Masud Haque[2], and Roderich Moessner[2] — [1]OIST, Okinawa, Japan — [2]MPI-PkS, Dresden

Loops are ubiquitous in physics, either as tangible entities such as polymers, or as emergent phenomena, especially where we do not expect them. In this talk, we shall focus on the latter case, where loops appear as extended degrees of freedom in spin ice crystals.

Spin ice has become a canonical member of the large and growing family of frustrated magnets, where excitations take the form of magnetic monopoles. The ground state of this system is highly degenerate and can be mapped exactly onto a fully packed loop model. We studied the statistics of this model both in 2 and 3 dimensions [1], making contact with Stochastic-Loewner Evolution processes (SLE), percolation and polymer physics, before illustrating implications of these results in related problems (Heisenberg magnets, itinerant electrons [2]).

[1] Jaubert, Haque, Moessner, PRL, 107, 177202 (2011)

[2] Jaubert, Pitaecki, Haque & Moessner, PRB, 85, 054425 (2012)

CPP 48.8 Thu 17:15 ZEU 250

**Membrane-driven collapse of DNA macromolecules and semiflexible filamentous virus particles** — Anastasiia B. Artemieva[1], Christoph Herold[2], Andrey G. Cherstvy[3], Petra Schwille[1], and •Eugene P. Petrov[1] — [1]Max Planck Institute of Biochemistry, 82152 Martinsried, Germany — [2]BIOTEC, Technische Universität Dresden, 01307 Dresden, Germany — [3]University of Potsdam, 14476 Potsdam-Golm, Germany

Interaction of (bio)macromolecules and colloidal particles with lipid membranes is one of the important problems of the modern bio-inspired soft matter physics. Earlier, we have found [1] that interaction of DNA molecules with strongly charged freestanding cationic lipid bilayers [2] leads membrane-mediated coil-globule transition of membrane-absorbed DNA macromolecules. Our recent experimental observations show that membrane-driven interactions at higher membrane charge densities are strong enough to induce the membrane-mediated collapse of much stiffer *fd* virus particles ($l_p \sim 2.2$ $\mu$m). We discuss these experimental findings in the framework of our new theoretical treatment [3] which takes into account membrane-polyelectrolyte electrostatic interactions, local membrane deformations, and polyelectrolyte bending rigidity.

[1] C. Herold, P. Schwille, and E. P. Petrov, *Phys. Rev. Lett.* **104** (2010) 148102.

[2] C. Herold, G. Chwastek, P. Schwille, and E. P. Petrov, *Langmuir* **28** (2012) 5518.

[3] A. G. Cherstvy and E. P. Petrov, *PCCP* (2014) in press.