BP 9: Posters: DNA & DNA Enzymes

Time: Monday 17:15–20:00 Location: P3

BP 9.1 Mon 17:15 P3

Formation of DNA Tubes and Attachment of Nanoparticles — Matthew Wiens, Awadesh Dwivedi, Nora Haufe, •Anja Henning, and Michael Mertig — Professur für Physikalische Chemie, Mess- und Sensortechnik, TU Dresden, 01062 Dresden

Synthesizing cylindrical nanostructures is an important goal in supramolecular chemistry, material science and nanotechnology. DNA is one of the most promising materials for such structures since its sequence can be designed to self-assemble into tubular structures through complementary base pairing. Different approaches have been reported showing DNA tube generation from either single stranded DNA or DNA building blocks, so called tiles [1]. Most of these methods have the drawback that side products such as 2D lattices are formed and the length of the structures periodically extend over tens of micrometers.

We used two-dimentional DNA origami procedure similar to Douglas *et al.* in order to create a six helix bundle with a well defined geometry [2, 3]. The design provides binding sites in periodic distances for functionalized nanoparticles. This is a promising feature for possible applications of future nanoelectronic and -photonic devices or a template for the investigation of biomolecules.

[1] Sharma et al., Science 323, 112-116 (2009) [2] Rothemund, Nature 440, 297-302 (2006) [3] Douglas et al., PNAS 104, 6644-6648 (2007)

BP 9.2 Mon 17:15 P3

Synthesis of covalently linked DNA structures — •Anja Henning[1,2], Ofer I. Wilner[2], Bella Shlyahovsky[2], Michael Mertig[1], and Itamar Willner[2] — [1]Professur für Physikalische Chemie, Mess- und Sensortechnik, TU Dresden, 01062 Dresden, Germany — [2]Institute of Chemistry and The Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

The ability of DNA as a material for bottom-up approaches has been shown already in an enormous number of experiments. Apart from some exceptions, the principle behind such DNA self-assemblies is the hybridization of complementary sequences through Watson-Crick base pairing which is unstable upon heating. We developed a new method to synthesize thermostable 2D and 3D DNA nanostructures by connecting single-stranded DNA (ssDNA) parts via covalent bonds. In order to demonstrate this approach, we used a ssDNA circle that contained four different internal modifications on its poles. These circles were cross-linked via the formation of covalent bonds with a ssDNA molecule that includes a modification on its 3‘ and 5‘ ends. We performed experiments using a circle with four amine functionalities and alternatively a circle, that contained thiol and amine functionalities at its opposite poles to yield DNA nanotubes. The single-stranded approach makes those structures suitable to guide patterning of nanoparticles, proteins and transition metals. Furthermore, the stability upon heating gives an outstanding erase/rewrite functionality, providing the possibility of a controlled release of the attached nanomaterials.

BP 9.3 Mon 17:15 P3

Die räumliche Synthese und Kodierung der DNA-Doppelhelix — •Norbert Sadler — 85540 Haar; Wasserburger Str. 25a

Es kann gezeigt werden, dass die räumliche DNA-Synthese sowie die Kodierung und Speicherung der Erbinformation durch eine räumliche Gruppen-Transformation der Basen- Tripletts und der assoziierten Aminosäure nach der harm. Streckenteilung erfogt. Die Transformation erfolgt über Drehspiegelung und Translation zwischen einem Ikosaeder und dem dualen Dodekaeder mittels lokaler Potentialfelder. Die Gruppe der 20 Basen-Triplette wird dabei aus den 60 Triplett-Kanten des 20-dreieckfläch. Ikosaeders gebildet, wobei die codierte Aminosäure mit dem zentralen C-Atom auf einem der 20 Ecken-Potentiale des Dodekaeders lokalisiert ist. Triplett und C-Atom bilden ein TranfertRNA Potential. Aufgrund der Pentagonstruktur erfolgt die Translation nach dem "Goldenen Schnitt"; Phi= 1,618. Am B-Typ der DNA kann dies bewiesen werden: Phi=(3,5nm;1Hel.Wind.+2,2nm;RNA-Abst.)/(3,5nm;1Hel.Wind.) Die Erbinformation und die Basensequenz kann in Form einer räumlichen Informationsspur auf und zwischen dem Dodekaeder und Ikosaeder, Computer unterstützt, zur Identifizierung der Primär-und Sekundärstruktur lokalisiert werden.

BP 9.4 Mon 17:15 P3

Information transfer and readout in complex DNA mixtures — •Harish Bokkasam and Albrecht Ott — Institute for Biological Experimental Physics, University of Saarland, Saarbruecken, Germany

Project: Development of an enzyme based method for the copy of oligos with predetermined length form biological template, given knowledge of the therein contained oligonucleotide sequence.

In this project, we modify the conventional PCR technique by using single primers to generate linearly amplified copies of single stranded oligos. This way the timescale of temperature cycle, which determines the length of the transcribed sequence is easier to control.

Results & Discussion: We find that single stranded DNA oligos of length b/w 40bp-200bp can be generated using this method. In order to determine the accuracy of the method the ssDNA is hybridised on a DNA coated surface with complementary sequence. We have shown that the time course of the hybridisation is almost identical to an error free sequence. This suggests the fidelity of the transcription.

Conclusion: Our method has given very promising results so far. Currently we are performing experiments along two lines: 1) Validate our technique by transcribing multiple single DNA sequences from a complex mixture. 2) Testing a different enzymes and polymerases for isothermal amplification and controlled extension of primers into short oligos. This will further improve the yield and also narrow the length distribution of the obtained products.

BP 9.5 Mon 17:15 P3

A Probabilistic Polymer Model for Mitotic Chromosomes — •Yang Zhang and Dieter W. Heermann — Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany

Despite many years of extensive studies the structure of the mitotic chromosome still remains unclear. The present work introduces a new probabilistic polymer model for mitotic chromosomes. The key assumption of the model is the ability of the chromatin fibre to crosslink to itself due to the dyanmic binding of proteins to the fiber. These protein-chromatin interactions were included by a probabilistic and dynamic mechanism. This is motivated by the observation of high repulsive forces between ring polymers. Computer simulations were performed to examine the validity of the model. Our results show that the presence of loops leads to a tight compaction and contributes significantly to the bending rigidity of chromosomes. Moreover, its qualitative prediction of the force elongation behaviour are close to experimental findings. The dynamic loop model indicates the crucial role of loops in mitotic chromosomes and a strong influence of their number and size on the mechanical properties. This shows that changes of these mechanical characteristics under different conditions can be explained by an altered loop structure.

BP 9.6 Mon 17:15 P3

Modelling the recruitment of DNA repair enzymes — •Gregor Weiss, Daniel Löb, and Barbara Drossel — Institut für Festkörperphysik, TU Darmstadt

We investigate the recruitment dynamics of repair enzymes during Base Excision Repair (BER) of DNA damage. Our focus lies on the possible competition of the enzyme loading platforms XRCC1 and PCNA in short patch BER. We also include Poly(ADP-ribose)polymerase-1 (PARP-1) in the model, which is indispensable for XRCC1 association with the DNA lesion.

We construct different possible models for the recruitment to DNA damage and dissociation of these three proteins, and perform numerical simulations of the models. In order to decide which models are more realistic, the simulation data are compared to empirical data obtained in living cells obtained using GFP-tagged proteins. Furthermore, these models are used to simulate the effect of protein inhibition, and to obtain more generally a relation between various model ingredients and signatures of the protein recruitment data curves.

BP 9.7 Mon 17:15 P3

Computer simulation of chromatin: Modeling the influence of nucleosome repositioning — •Oliver Müller[1], René Stehr[1], Robert Schöpflin[1], Ramona Ettig[2], Nick Kepper[2], Karsten Rippe[2], and Gero Wedemann[1] — [1]University of Applied Sciences Stralsund, 18435 Stralsund, Germany — [2]German Cancer Research

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The three-dimensional structure of chromatin is a key factor for controlling the DNA accessibility for protein factors, DNA replication and repair. However, it is still subject to extensive research since the interpretation of the experimental data is fraught with difficulties. Several structural models exist, many of which assume a strictly regular fiber. This regularity implies a highly periodical positioning as well as equal occupancy of the fiber nucleosomes, which is unlikely for *in vivo* chromatin. Recent studies indicate that only a small subset of nucleosomes seems to be strongly positioned whereas the majority of nucleosomes adhere to a statistical positioning mechanism. Other important factors, such as chromatin remodelers and transcription factors are also implicated in nucleosome repositioning and occupancy. Here, we carry out Monte Carlo simulations with a coarse-grained chromatin model incorporating elastic fiber properties as well as a detailed description of the electrostatic and internucleosomal interactions to investigate the effects of nucleosome repositioning. Depending on the extent of the displacements the fiber geometry changes significantly. This serves as a tentative explanation for the effects of different remodeling complexes on processes such as DNA transcription.

BP 9.8 Mon 17:15 P3

Dynamics of RNA based transcription control — •Michael Faber and Stefan Klumpp — Max Planck Institut für Kolloid- und Grenzflächenforschung Potsdam

Initiation of transcription is the main step at whcih gene expression is regulated. Bacteria often use a control mechanism called transcription attenuation that is at work immediately after the initiation of transcription. A transcribed sequence between the promoter and the coding region for the gene allows two, mutually exclusive structures the RNA transcript can form. The decision on whether transcription continues or is terminated, is made by choosing one of these structures which are therefore referred to as terminator and antiterminator. In recent years much efford has been expended to characterise such sequences. We have developed a structure-based model for studying the dynamics of RNA secondary structures, in particular, the dynamics of folding and unfolding of such competing structures. To simulate this dynamics, we use a Monte Carlo method with Metropolis rates, which are determined using the same parameters for the energy calculation as in models commonly used in RNA structure prediction like the individual nearest-neighbor model.

BP 9.9 Mon 17:15 P3

A unified model for statistical nucleosome positioning — •Brendan Osberg, Wolfram Moebius, and Ulrich Gerland — Ludwig Maximilians Universitaet, Munich, Germany

Recent genome-wide maps of nucleosome positions in different eukaryotes have revealed a common pattern around transcription start sites, involving a nucleosome-free region flanked by a pronounced periodic pattern in the average nucleosome density. For the yeast S. cerevisiae, a description of the periodic pattern has been established based on the statistical positioning mechanism of Kornberg and Stryer. This description derives from the physics of a dense one dimensional gas consisting of fixed-size particles. Here, we consider 12 Hemiascomycota yeast species, each of which displays a distinct nucleosome pattern. Since the chromatin constituents are highly conserved between species, and thus the mechanism underlying the formation of the patterns is expected to be related, we present a unified quantitative description.We extend the simple one-dimensional gas model account for transient unwrapping of short segments of nucleosomal DNA. Chromatin behavior in the majority of species is well described by this generalized gas model -only the average nucleosome density is a species-dependent variable. An exception is K. lactis, where we find an increased effective nucleosome width (potentially due to an increased use of linker histone H1 in this species). Together, our results provide a biochemically plausible role for nucleosome unwrapping in global chromatin behavior and establish a unified nucleosome gas model, providing a basis for quantitative analysis of chromatin effects on cis-regulatory transcription control.