BP 25: Posters: DNA/RNA and related enzymes

Time: Tuesday 14:00–16:00 Location: Poster A

BP 25.1 Tue 14:00 Poster A

Polymerization of RNA in a non-equilibrium environment — •Matthias Morasch, Christof B. Mast, and Dieter Braun — Systems Biophysics, LMU Munich, Germany

The polymerization of nucleotides to long chains of RNA was very likely a crucial step towards the evolution of life. There is, however, a large variety of possible nucleotides that require very different conditions in order to polymerize efficiently. These range e.g. from dry conditions at elevated temperatures to dry-wet cycles in lipid environments and to aqueous solutions in combination with a catalyst. We investigate different polymerization conditions for cyclic nucleotides, in particular 3',5'-cyclic guanosine monophosphate (cGMP), which might have the ability to polymerize in the dry state as well as in an aqueous environment. So far, we could proof that drying cGMP at elevated temperatures triggers its polymerization to 40 mers and longer.

While the drying process facilitates the formation of long polymers due to high local concentrations and the absence of water, a polymerization in an aqueous environment is a more cumbersome task. Especially the polymerization of pairing bases has to be accomplished for a prebiotic evolution. Theory shows that non-equilibrium conditions in form of a temperature gradient should allow the enhanced polymerization from cyclic nucleotides in a thermophoretic molecule trap. The local accumulation of monomers shift the polymerization towards ever longer RNA. It appears possible that RNA polymerization can be triggered using purely physical means without using any catalysts or highly tuned activation chemistry of the monomer.

BP 25.2 Tue 14:00 Poster A

Ultrafast energy dissipation within the vibrational modes of the DNA backbone — •Yingliang Liu, Biswajit Guchhait, Rene Costard, Torsten Siebert, and Thomas Elsaesser — Max-Born-Institut für Nichtlinear Opitk und Kurzzeitspektroskopie, Max-Born-Str. 2a, 12489 Berlin, Germany

The long-term stability of the DNA helix structure requires efficient processes of electronic and vibrational relaxation as well as energy dissipation into an aqueous environment. To determine the relevant time-scales and pathways of relaxation, femtosecond pump-probe experiments on artificial double-stranded DNA oligomers are performed under conditions of full hydration. Specifically addressing the structure of the DNA backbone in the frequency range from 950 to 1300 cm^{-1}, the vibrational modes of the phosphate group, phosphodiester linkage and the furanose ring structure display subpico- to picosecond lifetimes. While excess energy released by the relaxation of phosphate vibrations is preferentially transferred into the surrounding water shell, clear signatures of vibrational energy transfer to the modes of the sugar linkage and ring structure are observed and these channels of energy dissipation are compared for different hydration levels.

BP 25.3 Tue 14:00 Poster A

Ectoine induced water structuring as a possible explanation for radiation protection properties — •Marc Benjamin Hahn, Tihomir Solomun, Susann Meyer, Heinz Sturm, and Hans-Jörg Kunte — BAM - Federal Inst. Mater. Res., Berlin, Germany

Compatible solutes ectoine and hydroxyectoine are known to be effective protectant against heating, freezing, high salinity and radiation damage for biomolecules and cells. It is believed that this properties are due to water-structuring-effects and their influence on hydrogen-bonds within water-clusters and biomolecules. Although the beneficial properties of ectoine are already exploited in commercial applications the underlying mechanisms remain unclear. We propose an explanation for radiation protecion properties based on our findings from ramanspectroscopic measurements. We found changes of vibrational density of states in liquid water in dependence of ectoine, hydroxyectoine and sodium chloride concentrations. This data indicates linear increased collective behaviour of hydrogene bonds with compatible solute concentration which leads to higher scattering probablities of low energy electrons.

BP 25.4 Tue 14:00 Poster A

Compatible solute induced vibrational modes in water and the connection to radiation protection of biomolecules — •Marc Benjamin Hahn, Susann Meyer, Tihomir Solomun, Heinz Sturm, and Hans-Jörg Kunte — BAM - Federal Inst. Mater. Res., Berlin, Germany

Radiation protecion properties of compatible solutes are already exploited in medical applications. Even though the underlying mechanisms remain unclear. We present ramanspectroscopic measurements on the influence of the vibrational behaviour of water in dependence of compatible solutes concentrations. The results for ectoine and hydroxyectoine show an increase in the free density of states of the collective vibrational and the low frequency modes of water with increasing solute concentration. Based on this findings an explanation for the radiation protection properties will be proposed.

BP 25.5 Tue 14:00 Poster A

Uncovering the structural stability and unfolding pathway of a 7-bp DNA hairpin through high-temperature molecular dynamics simulation — •Ewa Anna Oprzeska-Zingrebe and Jens Smiatek — Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

The formation of specific DNA secondary and tertiary structures have been reported to play a key role in various range of biological processes, such as transcription termination or intermolecular binding. Among them, a pivotal role has been ascribed to DNA i-Motif and G-Quadruplex structures, which due to their biological appearance in telomeric and centromeric DNA are considered as potential targets for various diseases. Recent studies on high-temperature unfolding simulations of the DNA i-Motifs have revealed the existence of the stable hairpin configurations as an intermediate step in the unfolding pathway of DNA higher-order structures. In our study, we investigate simple 7-nucleotide DNA hairpin structures with the sequence d(GCGAAGC) and its variations. Through high-temperature molecular dynamics simulation we intend to get insight into the stability of the DNA hairpins and the possible unfolding pathways. In addition, the unfolding free energy landscape of DNA hairpins will be analyzed such that sequential differences can be energetically evaluated. This serves as the first approach to unravel the complex nature of G-Quadruplex folding pathway and behavior.

BP 25.6 Tue 14:00 Poster A

Measuring DNA translocation forces through various solid state nanopores with Optical Tweezers — •Sebastian Knust, Andy Sischka, and Dario Anselmetti — Experimental Biophysics & Applied Nanoscience, Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

We measured the forces acting on a single strand of dsDNA during translocation through nanopores in various solid state membranes by Optical Tweezers. The system includes a video-based force detection and analysis system allowing for virtually interference-free axial force measurements with sub-piconewton precision [1]. All measurements were performed with an overall force resolution of 0.5 pN at a sample rate of 123 Hz.

We show the controlled translocation through Si_2N_3 membranes both uncoated and lipid-coated [2]. Additionally, measurements of controlled dsDNA translocation through carbon nanomembranes (CNM) and through MoS_2 membranes were conducted.

Furthermore, measuring controlled translocation through graphene nanopores was found challenging, due to local heating phenomena encountered upon approaching an optically trapped microbead to a free standing graphene membrane. We analysed these phenomena in detail.

[1] S. Knust et. al., Rev. Sci. Instrum. **83**, 103704 (2012)
[2] L. Galla et. al., Nano Lett. **14**, 4176 (2014)

BP 25.7 Tue 14:00 Poster A

Modelling the mechanisms of backtrack and recovery in RNA polymerases I and II — Ana Lisica[1,2], Marcus Jahnel[1,2], Christoph Engel[3], •Edgar Roldan[4,5], Patrick Cramer[3], and Stephan Grill[1,2,4] — [1]BIOTEC, Technische Universität Dresden, Tatzberg 47/49, 01307 Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstrassüe 108, 01307 Dresden, Germany — [3]Max Planck Institute for Biophysical Chemistry, Am Fassberg 11, 37077 Göttingen, Germany — [4]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 81, 01187 Dresden, Germany — [5]GISC - Grupo Interdisciplinar de Sis-

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Transcription elongation by RNA polymerases is frequently interrupted by pauses. A prominent mechanism of pausing is backtracking, which involves backward movement of the polymerase on the DNA template. To recover from backtracks, polymerases can diffuse or cleave the backtracked RNA. We model the backtrack recovery of Pol I and II as a continuous time random walk between discrete states. We calculate the first-passage time from any position in the backtrack to the elongation competent state and compare it to times required for recovery from a given backtrack depth, as measured with high-resolution dual-trap optical tweezers. The choice of recovery mechanism is here determined by kinetic competition between 1D diffusion and transcript cleavage. Fitting experimental data to our model, we extract diffusion and cleavage rates of both enzymes and characterize the distinct micromehanical features of Pol I and Pol II transcription.

BP 25.8 Tue 14:00 Poster A

DNA hybridization and kinetics of hairpin-loop molecules — •Mina Mohammadi-Kambs, Björn Ackermann, and Albrecht Ott — Saarland university, FR 7.2, Biologische Experimentalphysik, 66123 Saarbrücken

In the cell, molecular information processing is based on molecular recognition and binding. Although DNA hybridization is sometimes understood as 'lock and key'. It is not clear how two molecules can identify each other. We find that there are many possibilities of different single strands of DNA at a given length that can bind to a given surface bound probe in thermal equilibrium. In other words, many keys can coexist for one lock. There are some groups of sequences, which do not bind to a probe like the ones with runs of guanine bases or self-complementary sequences. At the same time we look at the behavior of corresponding DNA hairpin-loop molecules. We investigate their thermal fluctuation by using a combination of fluorescence energy transfer and fluorescence correlation spectroscopy. We measure the rate of opening and closing for different sequences with different stem or loop length. In future work we will look at the behavior of DNA hairpin-loop molecule in the presence of competitive targets to see how they identify their complementary probe. This is a first approach towards understanding how molecular recognition works in the crowded and competitive environment of the cell.

BP 25.9 Tue 14:00 Poster A

Effects of Collectivity in Homology Recognition: a density functional theory based approach. — •Sergio Cruz[1], Claudia Danilowicz[2], Chantal Prevost[3], Mara Prentiss[2], and Maria Fyta[1] — [1]Institute for Computational Physics, University of Stuttgart, Germany — [2]Physics Department, Harvard University, Cambride, MA, USA — [3]LBT - CNRS and Univ Paris Diderot, Sorbonne Paris Cite, Paris, France

RecA is a family of proteins for performing homology recognition while trying to repair DNA. The atomistic mechanism by which this process occurs is not still fully understood. Crystallographic evidence shows that RecA separates a strand in sequences of three bases (triplet), and then searches for the homologous partner. However, 'recognition in duplets' is suggested as a possible mechanism by recent experiments. In our current investigation, the importance of collectivity in recognition is explored by means of quantum mechanical calculations at the level of dispersion corrected density functional theory. We compare the average binding energy for singlets, duplets, and triplets for canonical Watson-Crick and mismatched base pairs. There is a clear distinction between recognition in singlets, and recognition in duplets or triplets. We calculate the energy for duplets and triplets containing mismatches and compare this with the energetics of the respective singlets. Analysis on the energy difference will shed light to a better understanding of this homology recognition process.