

## BP 25: Focus: Charge Effects in Soft and Biological Matter I (joint CPP, BP, ST)

Time: Thursday 11:00–12:45

Location: H45

**Invited Talk**

BP 25.1 Thu 11:00 H45

**Charge effects in RNA folding** — •LOIS POLLACK — Cornell University, Ithaca, NY USA

Because nucleic acid backbones possess such a high negative charge, interactions with positively charged ions (or larger charged molecules) are critically important to the biophysics of both RNA and DNA. Our studies of the earliest events in RNA folding highlight the importance of electrostatic interactions to this conformational change. Complementary x-ray scattering experiments on short nucleic acid duplexes have elucidated the spatial distribution of condensed counterions, as well as ion-induced interactions between duplexes. Interactions between these helices can be tuned from repulsive to attractive by varying counterion charge and concentration. Interesting differences between RNA and DNA are revealed by these measurements.

BP 25.2 Thu 11:30 H45

**Dielectrophoresis: a new tool for continuous DNA/protein interaction studies** — •MARTINA EVERWAND, DARIO ANSELMETTI, and JAN REGTMEIER — Experimental Biophysics & Applied Nanoscience, Bielefeld University, Universitätsstr. 25, 33615 Bielefeld

The investigation of DNA-protein interactions is of central interest in today's proteomic research like for the metabolic pathway analysis. Here, a novel microfluidic device is presented, which allows efficient separation of protein-complexed DNA from native DNA strands in continuous mode.

The Lab-on-chip device consists of a 3D-structured microfluidic channel network incorporating an integrated barrier with nanometer dimension, that allows for electrodeless dielectrophoresis of DNA-protein complexes.

For the first time, we demonstrate that differently sized DNA fragments as well as DNA/protein and DNA/antibiotics complexes can be continuously separated from unbound DNA at a nano-microfluidic interface.

**Invited Talk**

BP 25.3 Thu 11:45 H45

**Origin of the electrophoretic force on DNA in solid-state nanopores** — •SERGE G. LEMAY — MESA+ Institute for Nanotechnology, University of Twente

Despite gel electrophoresis being one of the main workhorses of molecular biology, the physics of polyelectrolyte electrophoresis in a strongly confined environment remains poorly understood. Theory indicates that forces in electrophoresis result from interplay between ionic screening and hydrodynamics, but these ideas could so far be addressed only indirectly by experiments based on macroscopic porous gels. I will present a direct experimental based on measuring the electrophoretic force on a single DNA molecule threading through a solid-state nanopore as a function of pore size. The stall force gradually

decreases on increasing the nanopore diameter from 6 to 90 nm, inconsistent with expectations from simple electrostatics and strikingly demonstrating the influence of the hydrodynamic environment. We model this process by applying the coupled Poisson-Boltzmann and Stokes equations in the nanopore geometry and find good agreement with the experimental results.

BP 25.4 Thu 12:15 H45

**DNA Translocation through Nanopores: What is the role of dielectric permittivity?** — •STEFAN KESSELHEIM<sup>1</sup>, MARCELLO SEGA<sup>2</sup>, MEHMET SÜZEN<sup>3</sup>, and CHRISTIAN HOLM<sup>1</sup> — <sup>1</sup>Institut für Computerphysik, Universität Stuttgart — <sup>2</sup>Department of Physics and INFN, University of Trento — <sup>3</sup>Institute of Photonic Sciences, Castelldefels (Barcelona), Spain

We investigate the free energy barrier of a single DNA molecule filed through a synthetic nanopore. We employ a recently developed algorithm (ICC\*) that allows to take into account the dielectric contrast at the membrane/solute interface in coarse-grained molecular dynamics simulations. The investigations show the crucial contribution of dielectric mismatch to the translocation free energy barrier. We show that for low ionic strength and DNA fragments up to 100 bp the dielectric boundary forces dominate over the entropic contribution caused by DNA flexibility.

BP 25.5 Thu 12:30 H45

**DNA: charge localisation and pathogenesis.** — CHI-TIN SHIH<sup>1</sup>, YUN-YIN CHENG<sup>1</sup>, •STEPHEN A WELLS<sup>2</sup>, RUDOLF A RÖMER<sup>2</sup>, and CHING LING<sup>3</sup> — <sup>1</sup>Department of Physics, Tunghai University, 40704 Taichung, Taiwan and The National Center for Theoretical Sciences, 30013 Hsinchu, Taiwan — <sup>2</sup>Department of Physics and Centre for Scientific Computing, University of Warwick, Gibbet Hill Road, Coventry, CV4 7AL, UK — <sup>3</sup>Department of Physics, Chung-Yuan Christian University, Chung-Li, Taiwan

We present results from transfer-matrix modelling of charge localisation and transport in DNA sequences, using tight-binding models at several levels of detail. With parallel computing resources we are able to examine the variation in local charge-transport properties along sequences of hundreds of thousands of base pairs, covering entire genes. This has allowed us to survey large numbers of human genes for which databases of pathogenic mutations exist; we consider both cancer-related genes and those associated with other forms of genetic disorder.

Examining the correlations between charge transport (CT) properties and the sites where pathogenic mutations are observed, we find a statistically significant correlation between pathogenesis and below-average changes in CT properties. We discuss the interpretation of our results in the context of DNA physics and chemistry, and of possible cellular mechanisms for DNA damage avoidance, detection and repair.