MAR06-2005-006107

Abstract for an Invited Paper
for the MAR06 Meeting of
the American Physical Society

Microscopic Kinetics of DNA Translocation through Synthetic and Biological Nanopores

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Using highly focused electron beams, artificial pores of nanometer diameters can be manufactured in ultra-thin silicon membranes with a sub-nanometer precision. A trans-membrane voltage bias can drive DNA strands through such pores; the resulting electrical signals can be recorded. As the diameter of the pore as well as the thickness of the silicon membrane can be made to match precisely the dimensions of a DNA nucleotide, the electrical signals produced by the interaction of DNA with the pore were proposed to contain information about the DNA sequence. In order to relate the DNA sequence to the measured electrical signals we characterized DNA conformations inside the pore through molecular dynamics simulations. A typical simulated system included a patch of a silicon membrane dividing electrolyte solution into two compartments connected by the nanopore. External electrical fields induced capturing of the DNA molecules by the pore from the solution and subsequent translocation. To calibrate our methodology, we carried out MD simulations of DNA translocation through an α-hemolysin channel suspended in a lipid bilayer. Our results suggest that the rate-limiting step for DNA translocation through narrow synthetic pores is not the actual transit of DNA, but rather the search for such initial conformation that facilitates subsequent translocation. At the same time, hydrophobic adhesion of DNA bases to the pore walls may considerably slow down or halt DNA translocation. We observed a threshold electric field for translocation of double stranded DNA through pores smaller in diameter than a DNA double helix occurring due to the overstretching transition at load forces of $\sim$60 pN. In narrow pores, DNA bases were observed to tilt collectively towards the 5'-end of the strand, which explains experimentally observed directionality of single stranded DNA in the transmembrane pore of α-hemolysin.