Nanopores threading DNA: a multiscale approach

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Nanopores are nanometer sized pores, which are intensively investigated for their potential to be used as a very fast and cheap technology for sequencing DNA. In order to achieve this a nanopore is being used to electrophoretically thread DNA and the tunneling current across the nanopore is being used to read out the genetic information. Along these lines, we have applied different simulation schemes to unveil their properties. Using a multiscale methodology which couples the motion of the biomolecule with the surrounding ionic solution we were able to investigate the statistics and dynamics of the translocation of a biomolecule through a nanopore and describe a phenomenological model for the scaling law guiding this process. At a second step, we focus on the pore region and aim to optimize the sequencing abilities of a nanopore. For this, we have turned to the study of functionalized nanopores. In these, a functionalizing small molecule is attached on the nanopore surface and enhances the tunneling current signal. This electronic signal is used for distinguishing among the different DNA nucleobases and is essential for realizing a sequencing device. In the end, we discuss the electronic and transport properties of the functionalizing nanopores in view of their potential applications.