Supplementary Information on "DNA Translocating through a Carbon Nanotube Can Increase Ionic Current"

Jae Hyun Park^{1,2}, Jin He^{3,4}, Brett Gyarfas⁴, Stuart Lindsay^{4,5,6}, and Predrag S. Krstić^{1,7,8}*

¹Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, ²Department of Aerospace and System Engineering, Gyeongsang National University, Jinju, Gyeongnam 660-701, South Korea, ³Physics Department, Florida International University, Miami, FL 33199, ⁴Biodesign Institute, ⁵Department of Physics, ⁶Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287, ⁷Joint Institute of Computational Science, University of Tennessee, Oak Ridge, TN 37831, USA, ⁸Depaqrtment of Physics and Astronomy, University of Tennessee, Knoxville, TN 37006, USA

* To whom correspondence should be addressed: Predrag S. Krstić (pkrstic@utk.edu)

We present two representative movies (movie1.mpg and movie2.mpg) for the motions of solvated ions (K⁺and Cl⁻) and DNA in SWCNT with and without DNA. In the movies, the total surface charge on the CNT wall is Q = -1e while the magnitude of mobile charge is q = -0.4e, and the applied external electric field is $E_{ext} = 0.2$ V/nm. The time duration of movies is 1.25 ns. The cations are presented by dark blue, while the anions are of the light green color.

The comparison of two movies illustrates the mechanism of current enhancement in the presence of DNA. As seen in dna.mpg, after transient period (< 0.75 ns) the DNA "sits" at the exit end of SWCNT, filtering Cl⁻ ions. This produces a significant increase of electro-osmotic current through CNT due to larger excess charge inside the tube. For the last 0.5 ns of the movie with DNA (movie2.mpg), nine K⁺ pass through the CNT whereas all the Cl⁻ ions are blocked out by the DNA. This corresponds to the ionic current of 2.9 nA. However, in the same case but without DNA (movie1.mpg) the motion of ions inside tube is too slow to provoke a significant ionic current because the excess charge is small. Namely, one can observe the considerable amount of Cl⁻ ions inside the tube moving in the same direction as the cations (K⁺) which are induced by the negative surface charge of the CNT.