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**Monitoring DNA polymerase with nanotube-based nanocircuits**

YAN LI, MIROSLAV HODAK, WENCHANG LU, JERRY BERNHOLC, North Carolina State University, PHILIP COLLINS, University of California Irvine — DNA polymerases play an important role in the process of life by accurately and efficiently replicating our genetic information. They use a single-stranded DNA as a template and incorporate nucleotides to create the full, double-stranded DNA. Recent experiments have successfully monitored this process by attaching a Klenow fragment of polymerase I to a carbon nanotube and measuring the current along the tube [1]. Follow-up experiments have shown promise for distinguishing between DNA base pairs when nucleotide analogs are used [2], thus opening a new avenue for DNA sequencing. In this talk, we present results from computational studies on DNA polymerase I nanocircuits. The enzyme was first equilibrated in molecular dynamics and then density functional theory and Keldysh non-equilibrium Green's function methods were used to calculate the ballistic transmission coefficients and currents for different enzymatic states. Our results show significant change in current when the enzyme alternates between open (idle) and closed (synthesizing) states. We can also differentiate between some template bases when modified nucleotides and gate scanning are used. [1] T. J. Olsen et. al., JACS 135, 7855 (2013) [2] K. M. Pugliese et. al., JACS 137, 9587 (2015)

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