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Computational investigation of CNT-based DNA polymerase nanocircuits YAN LI, MIROSLAV HODAK, WENCHANG LU, JERRY BERNHOLC, North Carolina State University, PHILIP COLLINS, University of California Irvine — DNA polymerases are important enzymes that replicate DNA molecules with very low error rates – about one error in 10^5 bases. Recently, it was found that the replication process can be electrically monitored by attaching a Klenow fragment of polymerase I to the surface of a carbon nanotube and monitoring the current along the tube [1]. In this talk, we report results from computational studies on DNA polymerase nanocircuits. We have first performed classical molecular dynamics (MD) calculations to get snapshots of different enzymatic stages, particularly the open state (no DNA binding) and the closed state (DNA double helix binding). We then used density functional theory (DFT) and Keldysh non-equilibrium Green's function (NEGF) formalism to calculate transmission coefficients and currents for each enzymatic state. Our results show that the transmission spectrum and the currents change significantly when the enzyme moves from the open to the closed state. While the initial experiments did not show signal differences between dissimilar bases, the theoretical work in progress is investigating conditions where bases might have distinct signatures, which would allow for DNA sequencing.

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