Quantum transport studies of CNT-Based DNA Polymerase Nano-Circuits

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DNA polymerases are important enzymes that replicate double-helix DNA from single stranded template with both very high replication rate, hundreds of bases per second, and very low error rate, one per ~10^5 bases. Recently, it was found that the replication process can be electrically monitored by attaching a "Klenow fragment" (KF) of *polymerase I* to the surface of a carbon nanotube (CNT) and monitoring the current through the nanotube during replication. In this presentation, we report results from computational studies of DNA polymerase nano-circuits. We have first performed classical molecular dynamics simulations to obtain snapshots of different enzymatic stages, particularly the *open* state (when the enzyme is not replicating) and the *closed* state (when the enzyme is synthesizing a new base pair). We then used density functional theory and Keldysh non-equilibrium Green's function formalism to calculate transmission coefficients and currents for different enzymatic states. Our calculations show that the transmission spectrum and the current change significantly when the enzyme moves from the open to the closed state. While the original CNT-KF setup did not find significant differences between dissimilar bases, our theoretical work shows that both nucleotide analogs and gate potential scanning help distinguish between different DNA bases. Current work in progress is investigating conditions in which different bases might show larger variations in currents, which would allow for electrical sequencing of DNA.