Electronic Supplementary Material (ESI) for Nanoscale Advances.

Supporting Information

Functionalized Carbon Nanotube Electrodes for Controlled DNA Sequencing

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Table S1. Binding energy (E_b, in eV) for the pristine and functionalized closed-end cap CNT (6,6) with purine and pyrimidine type molecules.

Probe/Target Nucleotide	dAMP	dGMP	dTMP	dCMP
Pristine CNT	-0.69	-1.01	-0.68	-0.40
A-probe	-1.40	-1.61	-1.65	-0.62
G-probe	-1.90	-2.35	-1.53	-2.08
T-probe	-1.60	-1.91	-1.50	-1.21
C-probe	-1.50	-2.31	-1.36	-1.50

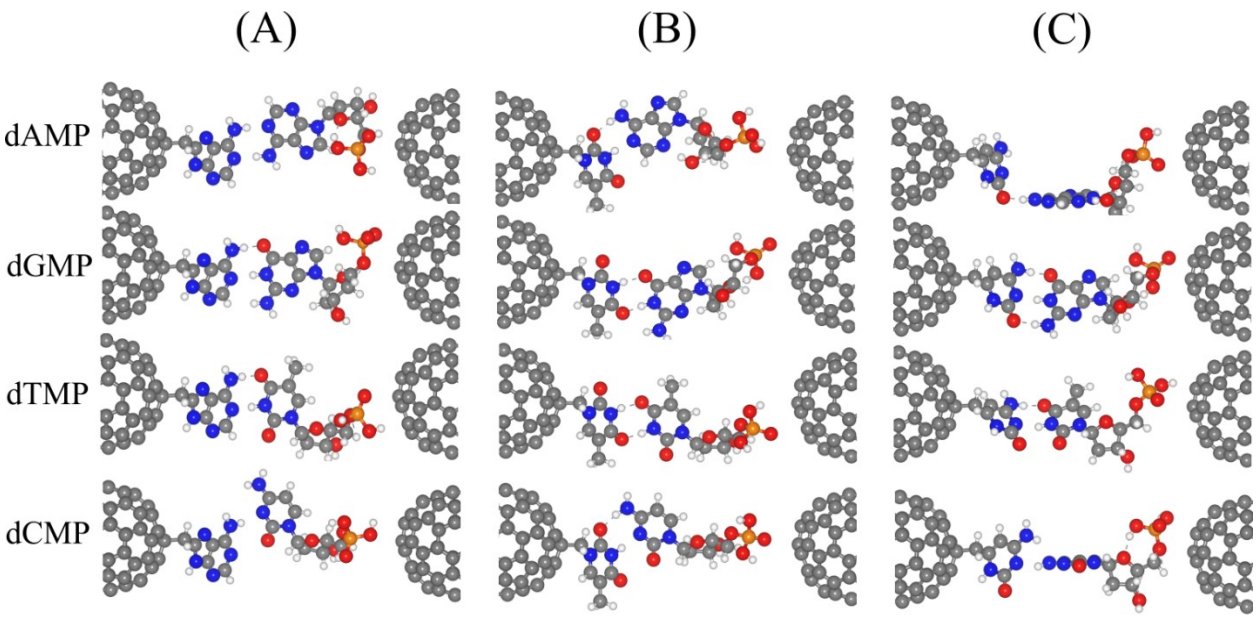

Figure S1. The fully optimized functionalized closed-end cap CNT (6,6) nanogap setup for measuring the transmission and $I-V$ curves of the four target DNA nucleotides: dAMP, dGMP, dTMP and dCMP are presented. The CNT electrodes are functionalized by a reader-nucleobase [(A) Nanogap setup with A-probe; (B) Nanogap setup with T-probe; and (C) Nanogap setup with C-probe; respectively].

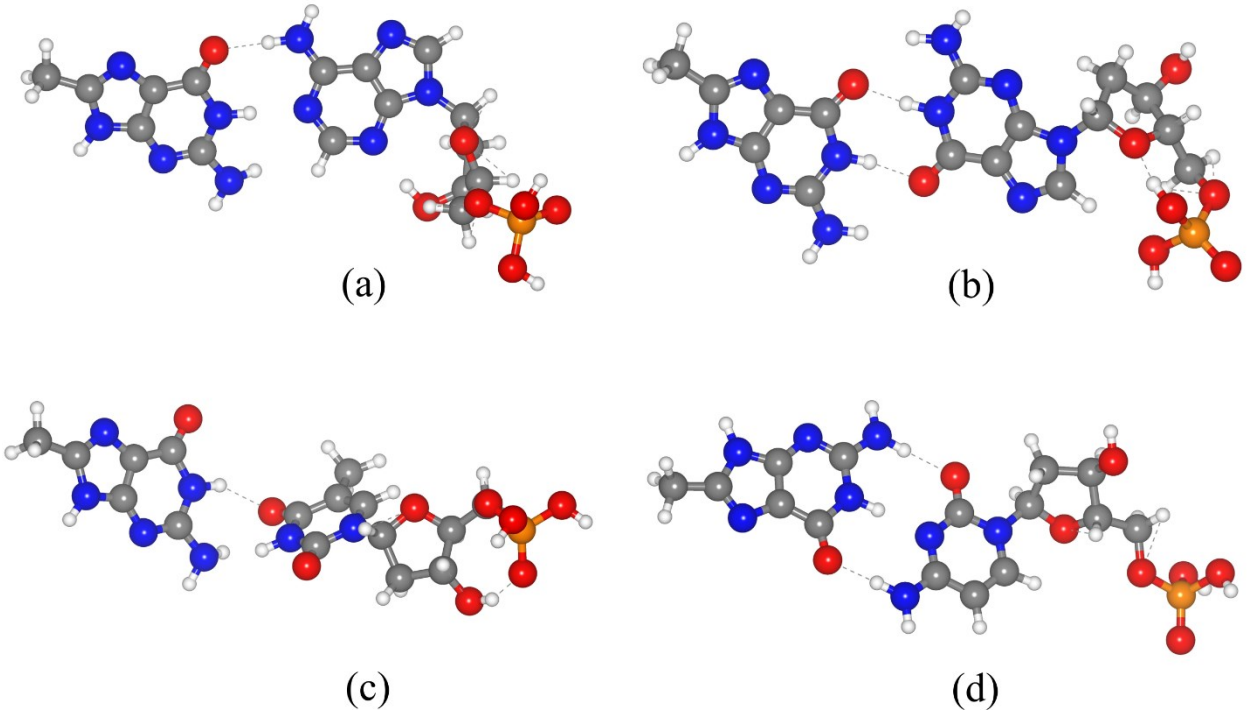

Figure S2. Optimized reader-target pair geometries: (a) G-dAMP, (b) G-dGMP, (c) G-dTMP, and (d) G-dCMP.

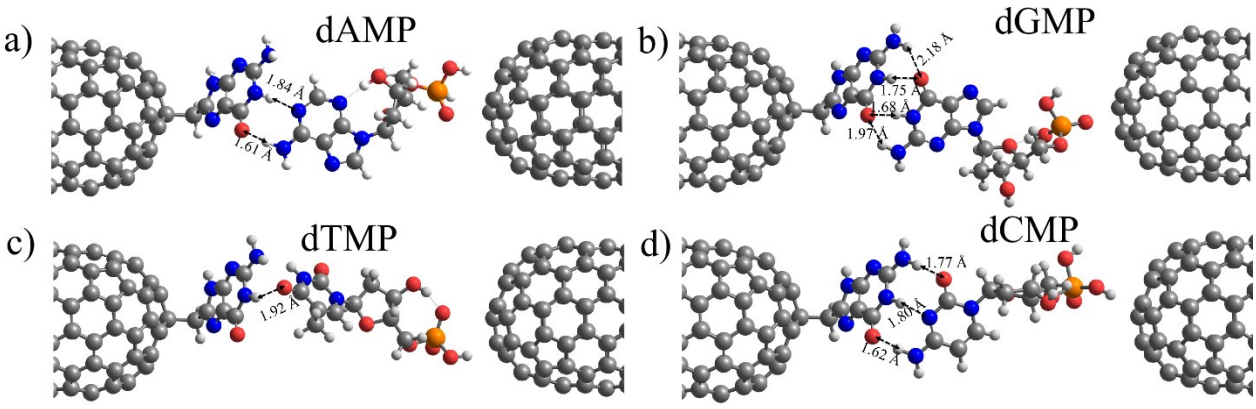

Figure S3. (a-d) Most stable configurations for the four nucleobases dAMP. dGMP, dTMP, and dCMP.

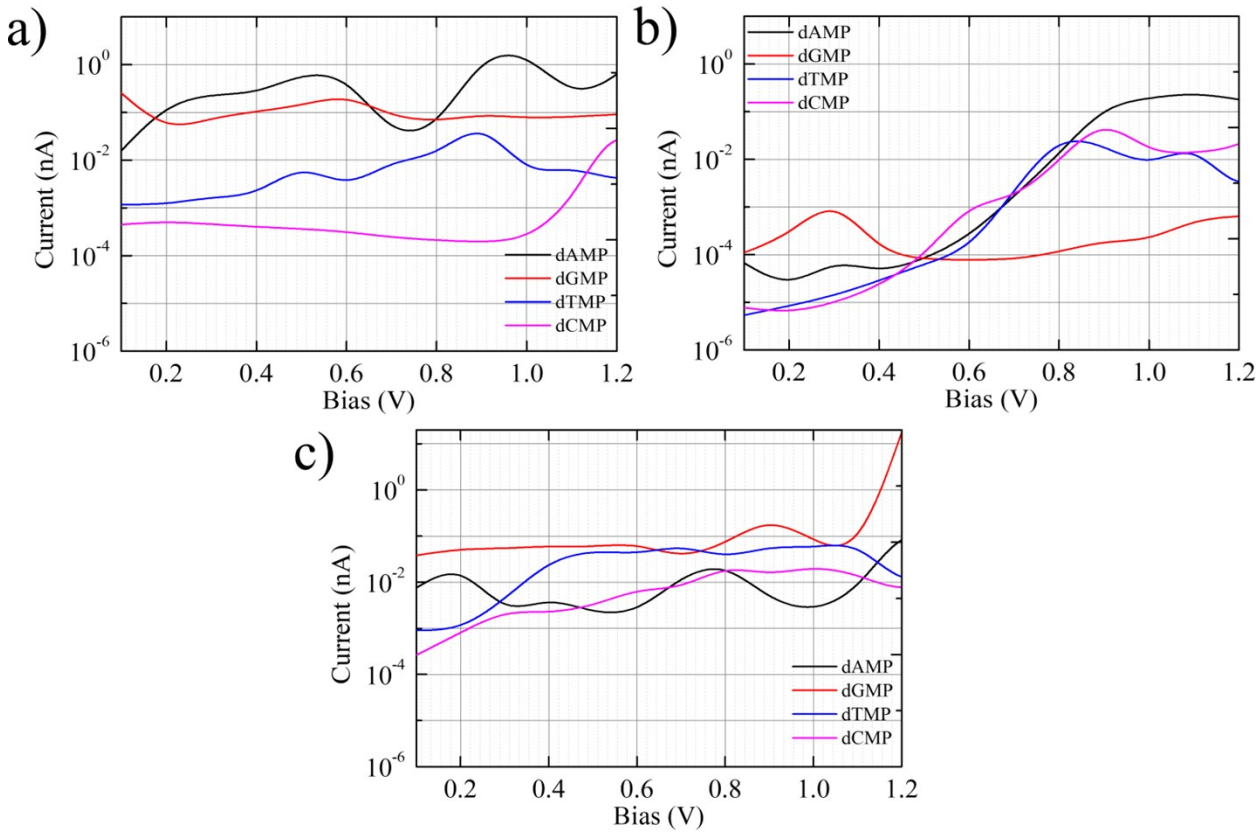

Figure S4. The $I-V$ characteristic curves plotted on a semi-logarithmic scale for all four target nucleotides (dAMP, dGMP, dTMP, and dCMP). (a) Nanogap setup with adenine-probe; (b) Nanogap setup with thymine-probe; and (c) Nanogap setup with cytosine-probe.

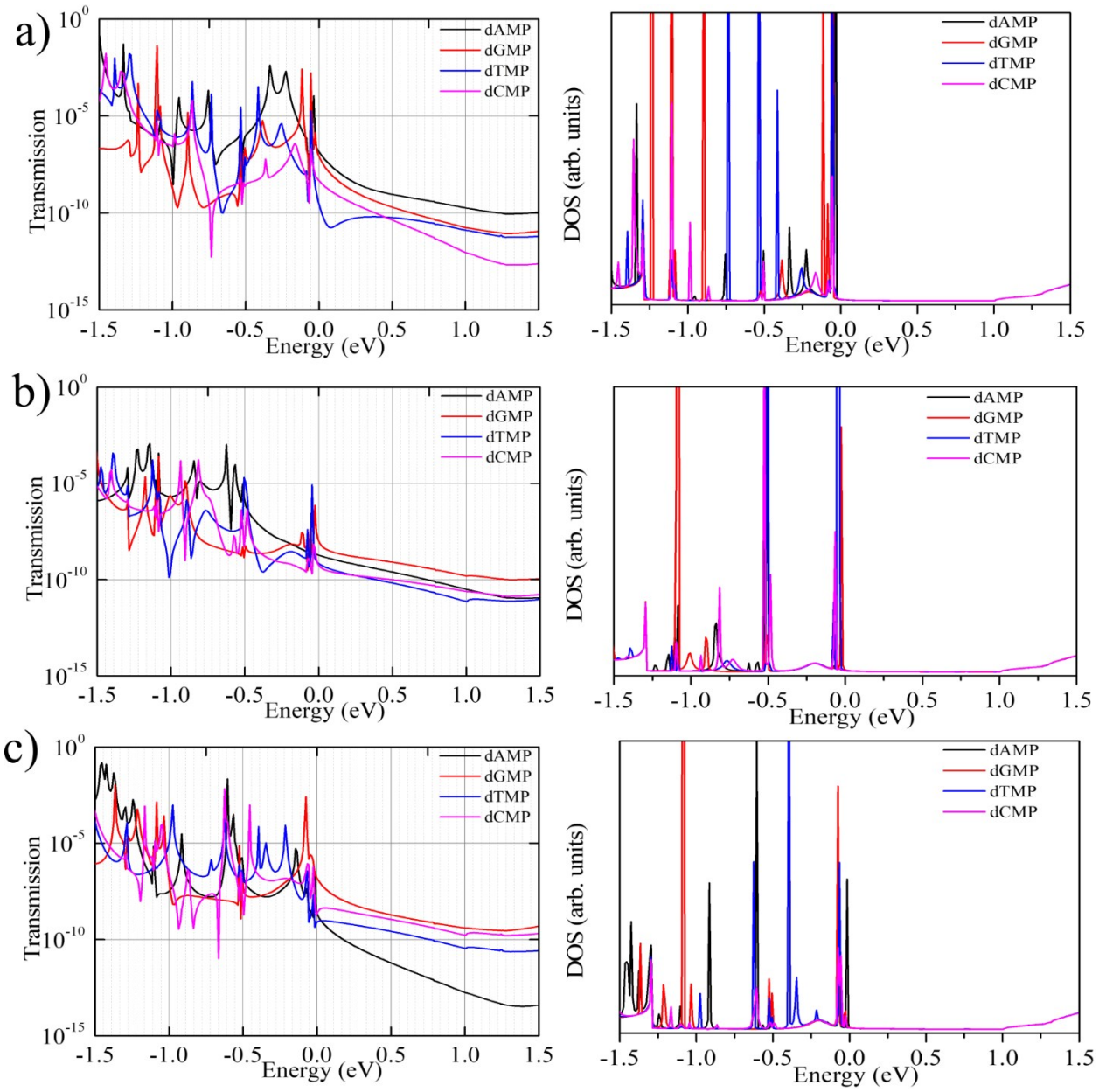

Figure S5. In the right panel, the zero-bias transmission function plotted on a semi-logarithmic scale for all four target nucleotides (dAMP, dGMP, dTMP, and dCMP) is presented. (a) Nanogap setup with adenine-probe; (b) Nanogap setup with thymine-probe; and (c) Nanogap setup with cytosine-probe. In the left panel, the zero-bias DOS plotted for all four nucleotides. The Fermi-level has been aligned to zero energy.

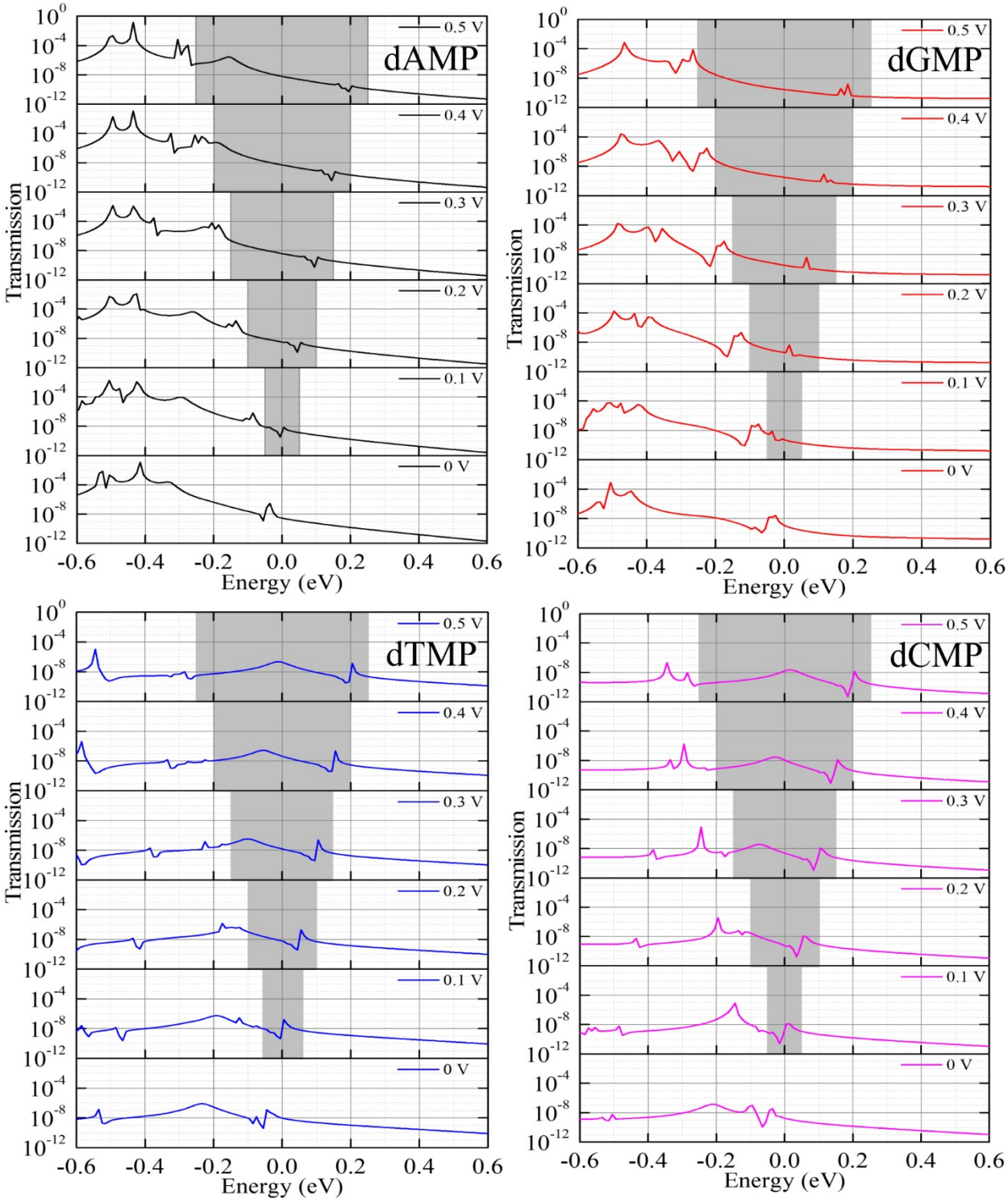

Figure S6. Nanogap setup with Guanine-probe. The bias-dependent transmission functions plotted on a semi-logarithmic scale for all four target nucleotides (dAMP, dGMP, dTMP, and dCMP), with variation of energy E at different bias voltages (0.0-0.5 V). The grey shaded area represents the bias voltage window of ±V/2.

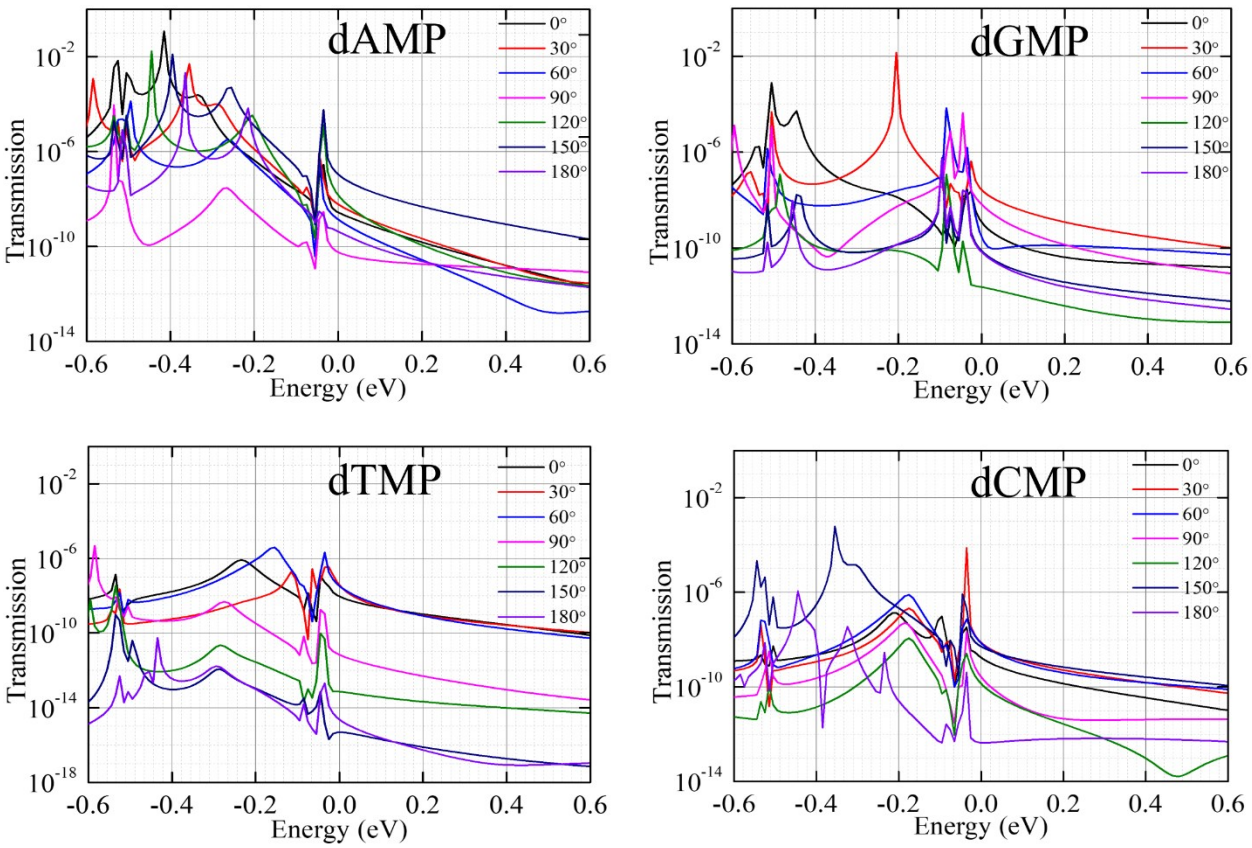

Figure S7. Zero-bias transmission functions plotted on a logarithmic scale of all the four nucleotides (dAMP, dTMP, dGMP, dCMP) for the guanine-probe functionalized CNT nanogap in xy-plane rotated around z-axis in the steps of 30° with respect to their original positions.

Effect of Different Types and Radiuses of the CNTs Electrodes on Transmission Function:

We have considered two more nanogap setups: (i) one with armchair CNT (4,4) and (ii) another with zigzag CNT (6,0) electrodes functionalized with a guanine probe to investigate the transmission function. Each electrode have 48 atoms in left and right side and the scattering region lengths are 4.48, 5.51, and 5.59 nm for CNT (6,6), CNT (4,4), CNT (6,0); respectively. The proposed nanogap setups for guanine functionalized closed-end cap armchair CNT (6,6), armchair CNT (4,4), and zigzag CNT (6,0) are shown in **Figure S8**.

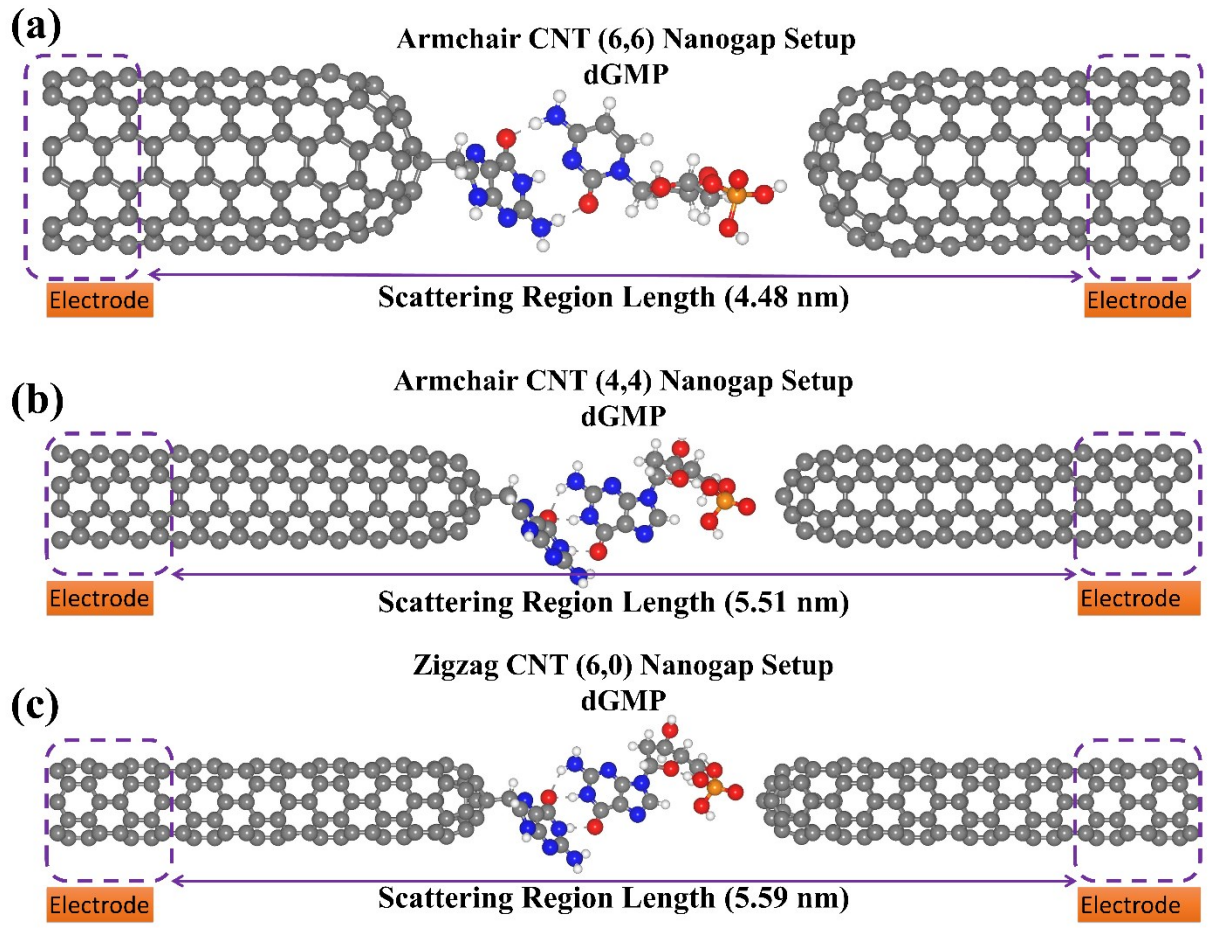

Figure S8. The fully optimized guanine-probe functionalized closed-end cap (a) armchair CNT (6,6), (b) armchair CNT (4,4), and (c) zigzag CNT (6,0) nanogap setup for measuring the transmission of the four target DNA nucleotides: dAMP, dGMP, dTMP and dCMP are presented.

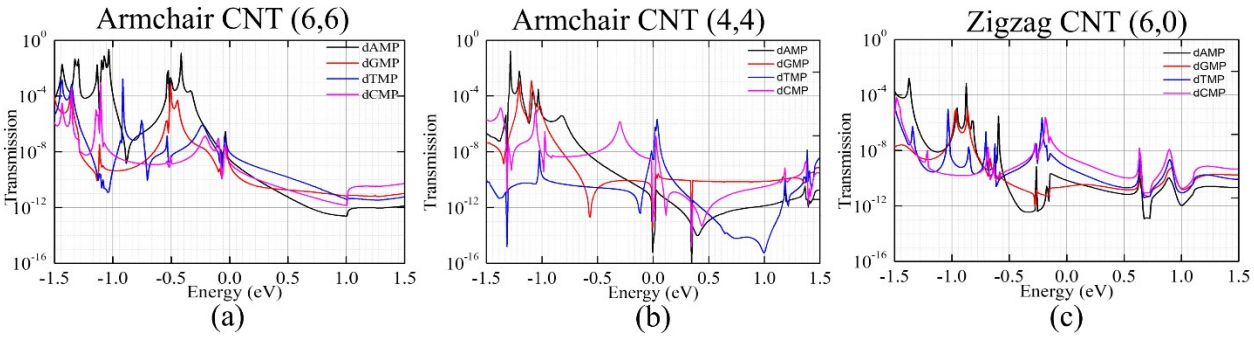

Figure S9. The zero-bias transmission function calculated for a guanine-probe functionalized closed-end cap (a) armchair CNT (6,6), (b) armchair CNT (4,4), and (c) zigzag CNT (6,0), respectively.