Supporting information for: Controlled current confinement in interfaced 2D nanosensor for electrical identification of DNA

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In this support information we provide the map of the charge density and wave function redistribution for each natural nucleobase (dAMP, dGMP, dCMP and dTMP) inside our nanopore device by comparing the total charge of each system with their separated parts.

1 Charge density difference:

The charges density redistribution are shown in figure 1 a-d, for dAMP, dGMP, dCMP, dTMP, respectively. The definition is given by the total charge density between the fully system (DMD + DNA), minus the counterparts separated as the following:

$$\rho_{diff}(r) = \rho_{DMD+DNA}(r) - (\rho_{DMD}(r) + \rho_{DNA}(r)) \quad (1)$$

The ρ_{diff} indicates how the charge is redistributed in the system due to DNA pore interaction. The positive ($\rho_{diff} > 0$) charge difference is represented by orange and the negative one ($\rho_{diff} < 0$) by red color.

2 Wave function:

The wave function are shown in figure 2 a-d for dAMP, dGMP, dCMP, dTMP, respectively. We note for the energy (E=-0.18 eV), the electron probability are bigger in the lower carbon nanowire, as expected. These results are corroborating with the local current shown in the main paper.

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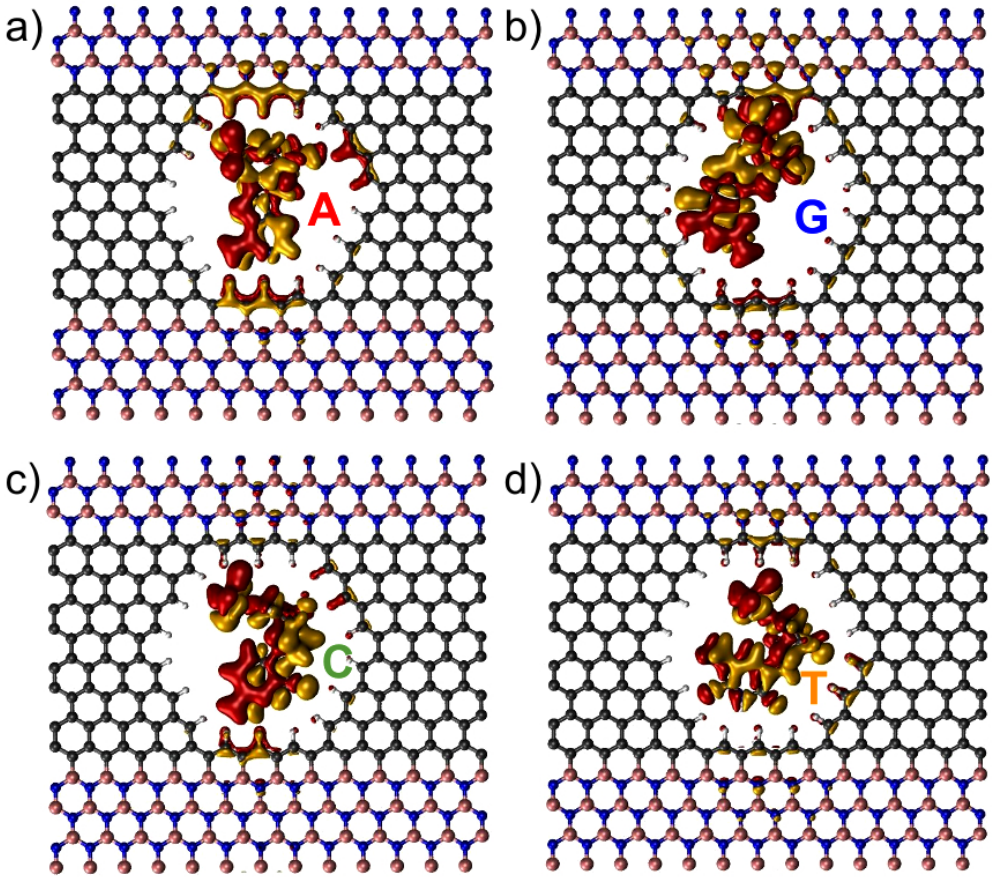

Fig. 1 Charge density difference plots for a) dAMP, b) dGMP, c) dCMP and d) dTMP.

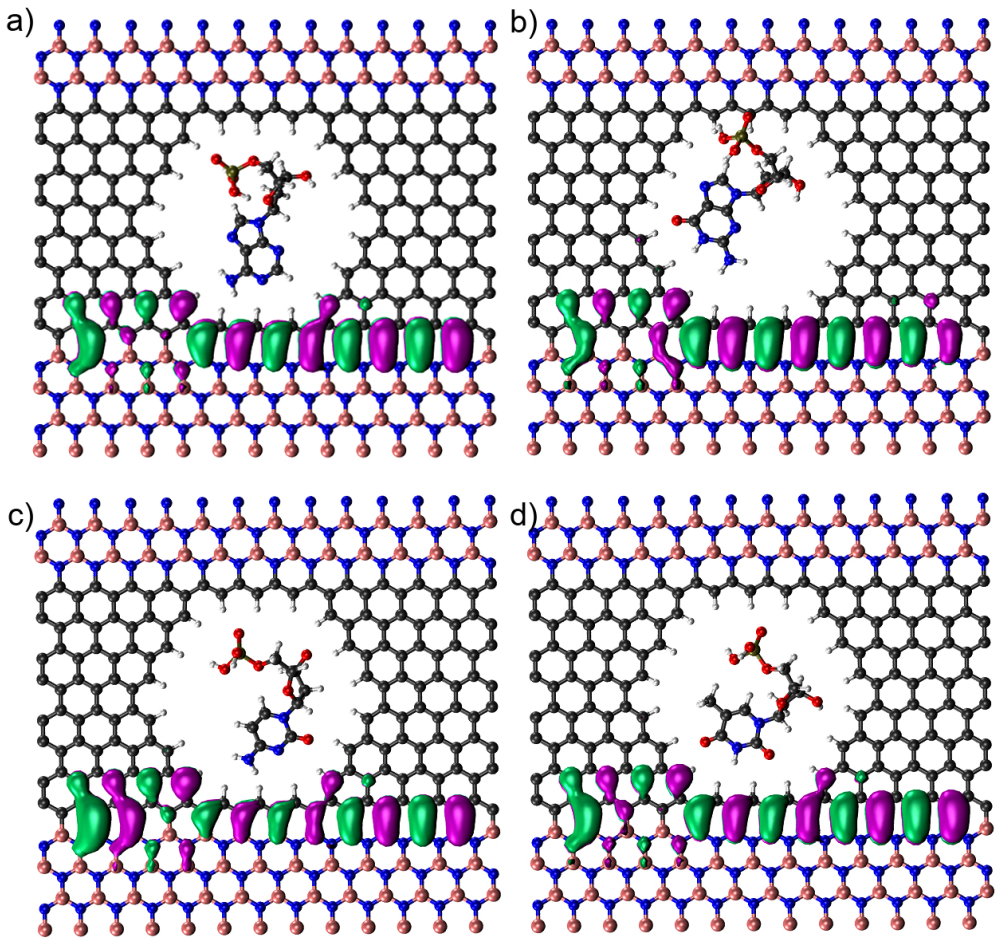

Fig. 2 Wave function plots for E=-0.18 eV are shown in each panel as the following: a) dAMP, b) dGMP, c) dCMP and d) dTMP.