Electronic Supplementary Information for

"DNA/RNA Sequencing Using Germanene Nanoribbons via Two Dimensional Molecular Electronics Spectroscopy: An ab initio Study"

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Charge density redistribution

To provide a better vision on the nature of the interaction between nucleobases and AGeNR, we plot the isosurfaces of the calculated spatial charge density difference for all nucleobases adsorbed onto the AGeNR's surface. To this end, the following equation is used to calculate the the change in charge density:

$$\Delta\rho(\vec{r}) = \rho_{AGeNR+base}(\vec{r}) - \rho_{AGeNR}(\vec{r}) - \rho_{base}(\vec{r})$$

where $\rho_{AGeNR+base}(\vec{r})$, $\rho_{AGeNR}(\vec{r})$, and $\rho_{base}(\vec{r})$ are the charge density of nucleobase-AGeNR system, AGeNR, and nucleobase respectively. Fig. S1 depicts the resulting isosurfaces of the calculated spatial charge density redistribution for the studied nucleobaseAGeNR systems. Red/blue color represents positive/negative values of $\Delta\rho(\vec{r})$ indicating the decrease/increase in the charge density of the region. It can be seen from the plotted isosurfaces that charge redistribution is mainly concentrated to the nucleobases and there is no complex redistribution of charge density between nucleobases and AGeNR. This is also confirmed with our Bader charge analysis which does not show explicit charge transfer between nucleobases and AGeNR. It means that the interaction of nucleobases with AGeNR has the physisorption nature and is madiated by weak vdW forces .

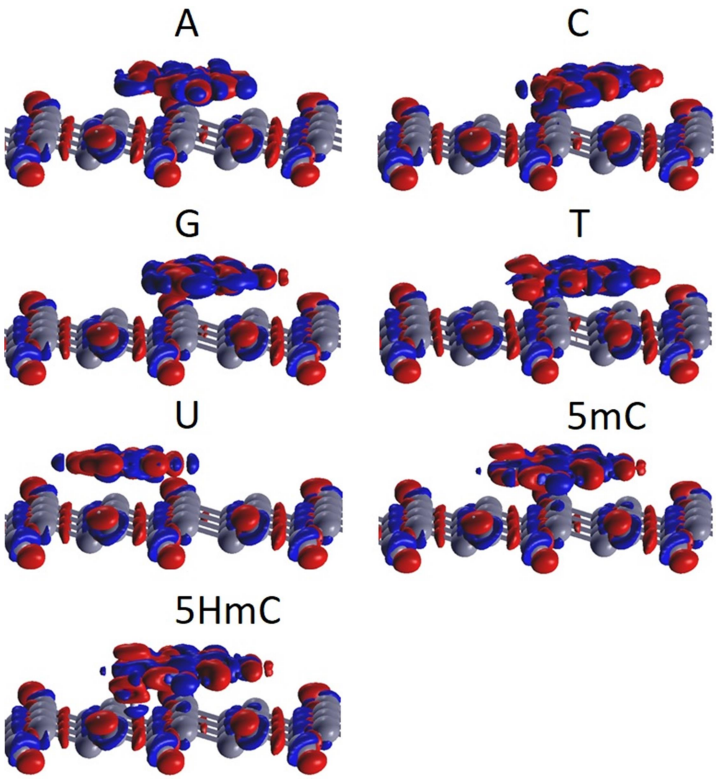

Fig. S1 Spatial charge density redistribution of different nucleobase-AGeNR systems. The isovalue is 0.006 a.u. Red/blue color represents positive/negative values of $\Delta\rho(\vec{r})$ indicating the decrease/increase in the charge density of the region. Ge atoms are presented in gray color.

Current-voltage profiles of nucleobase-AGeNR systems

Here, we represent the calculated current-voltage (I-V) profiles of the studied nucleobase-AGeNR complexes to compare the capabilities of 1D current measurement and 2DMES technique in unambiguous discrimination of various nucleobases using emerged electronic molecular fingerprints. Fig. S2 illustrates the I-V curves of different nucleobase-AGeNR systems for two applied gate voltages of V_g = 0.5 V and 1 V. The plotted I-V curves show that although at some gate voltages, distinguishing some nucleobases from each other with an acceptable resolution might be possible, however the molecular differentiation of all nucleobases would be struggling at some other gate voltage values. This indicates that 1D current measurement at zero or single gate voltage would not be adequate for unambiguous recognition of all nucleobases. Therefore, it is required to sweep V_g in a certain window to provide a conductance map for every nucleobase, as is performed in 2DMES technique, for a high resolution molecular recognition.

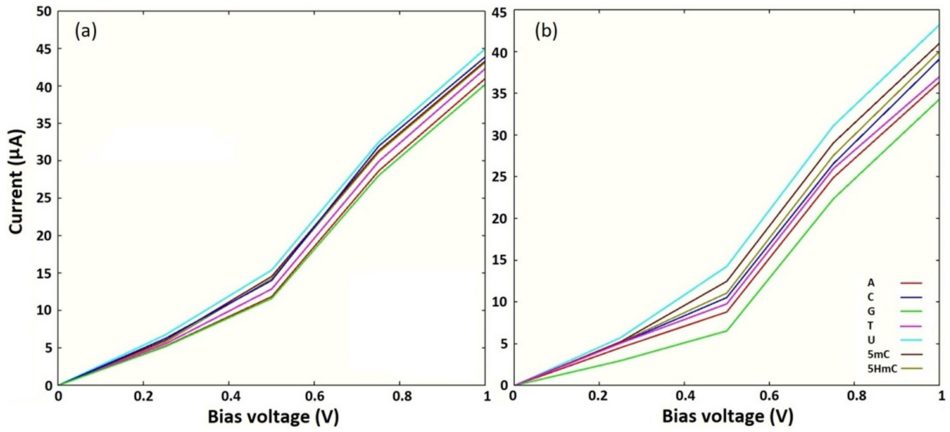

Fig. S2 Current-voltage profiles of different nucleobase-AGeNR systems for two gate voltages of (a) V_g = 0.5 V and (b) V_g = 1 V.