Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

DNA sequencing based on electronic tunneling in gold nanogap: a first-principles study

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Atomic structure of Gap-Au

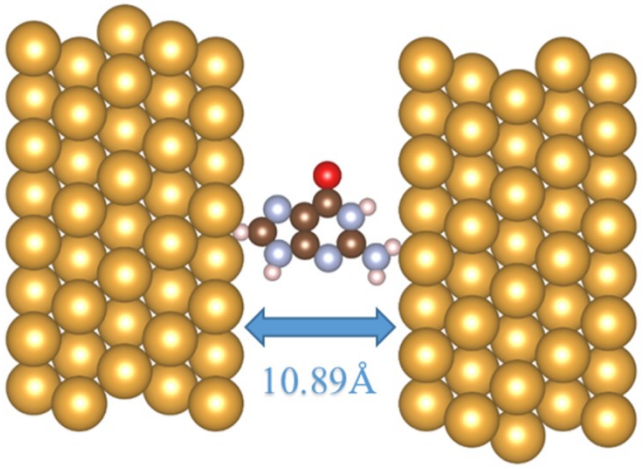

Fig. S1 The atomic structure of the bare gold nanogap, with a gap size of 10.89 Å.

Table S1. Average currents of nucleobases in the three nanogaps

I (nA)	Gap-Au	Gap-AuS	Gap-AuS’
G	4.761E-01	1.148E+00	3.164E-02
A	9.741E-02	3.939E-02	4.710E-04
C	3.180E-01	3.673E-01	5.264E-03
T	1.092E-01	2.815E-03	7.693E-06

Effect of gap size on total energy for Gap-AuS

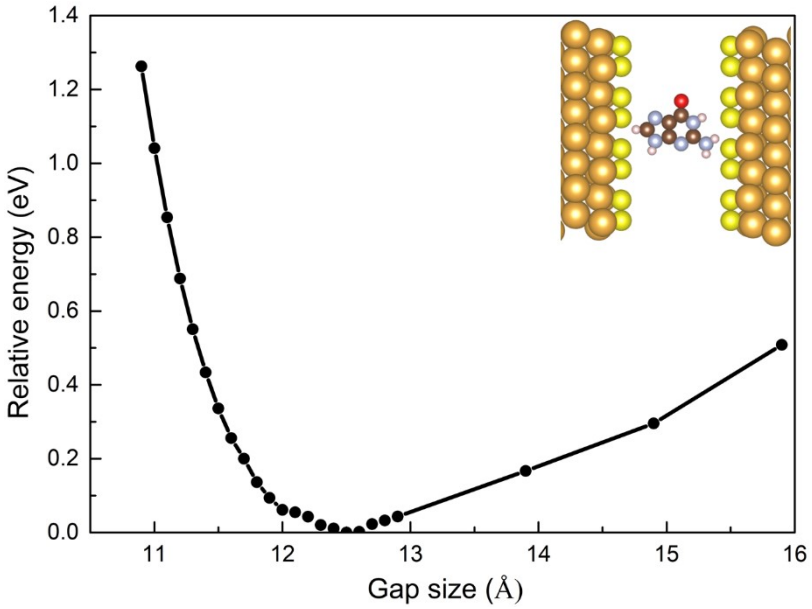

Fig S2. Total energy of Gap-AuS versus nanogap size.

We keep the orientation of guanine in Gap-AuS with the highest conductivity and vary the size of nanogap. We denote the nanogap as Gap-AuS' where the system is found to be most stable. Fig S2 plots the total energy as a function of the nanogap size and the minimum energy is found when the gap size is 12.49 Å. In this way, we maximize the residence time of guanine with the highest conductivity in Gap-AuS'.

Electronic transport properties of Gap-AuS’

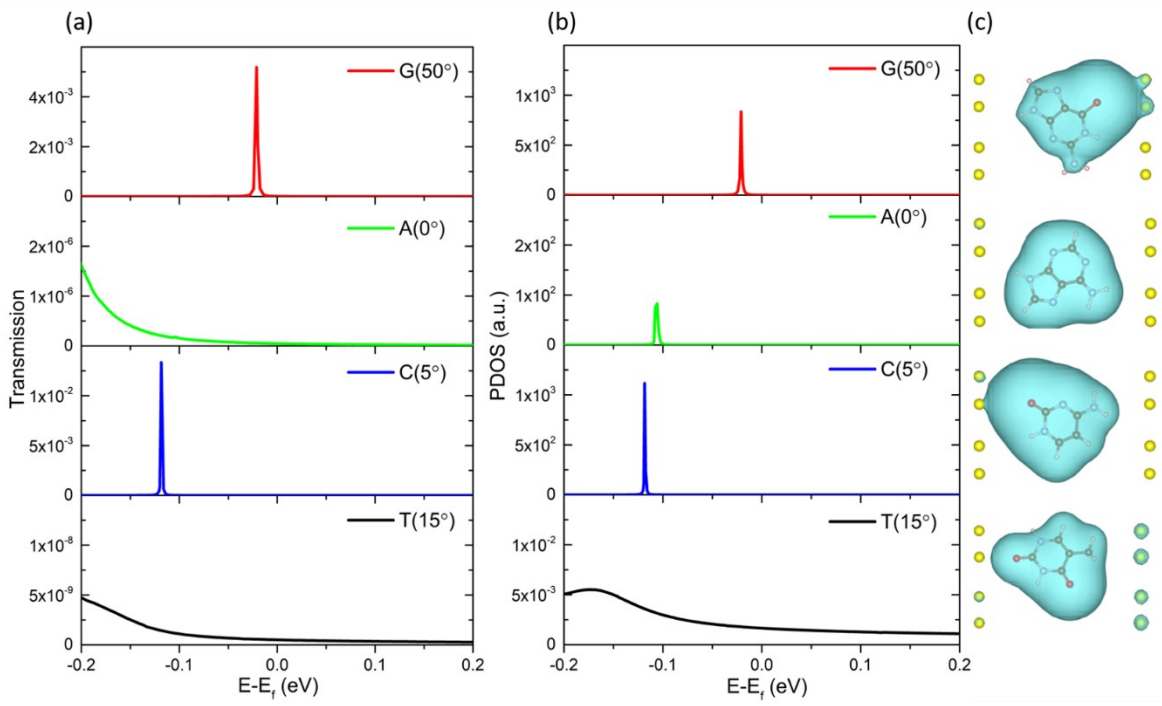

Figure S3. Transmission coefficients (a) and PDOS (b) of each nucleobase in Gap-AuS’. DOS of electrodes is excluded for clarity. For each nucleobase, the orientation with the largest contribution to the average current is chosen for the analysis. (c) Isosurface plots of HOMOs of the four nucleobases with the nanogap.

Difference in electrostatic energy between Gap-Au and Gap-AuS

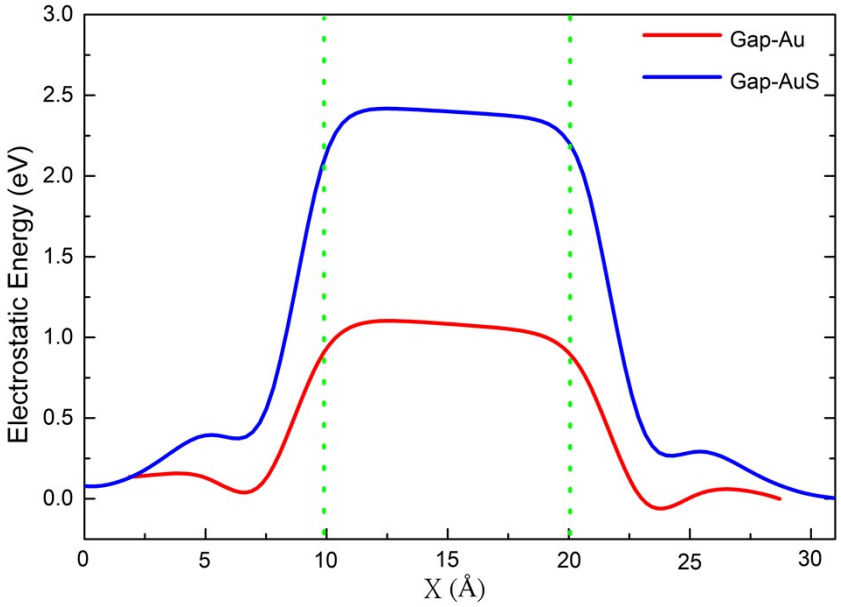

Fig S4. Electrostatic energy of Gap-Au (red line) and Gap-AuS (blue line), without nucleobase in the nanogap. The X axis indicates the direction of the electron transport, and the green dashed lines mark the edge of electrodes.

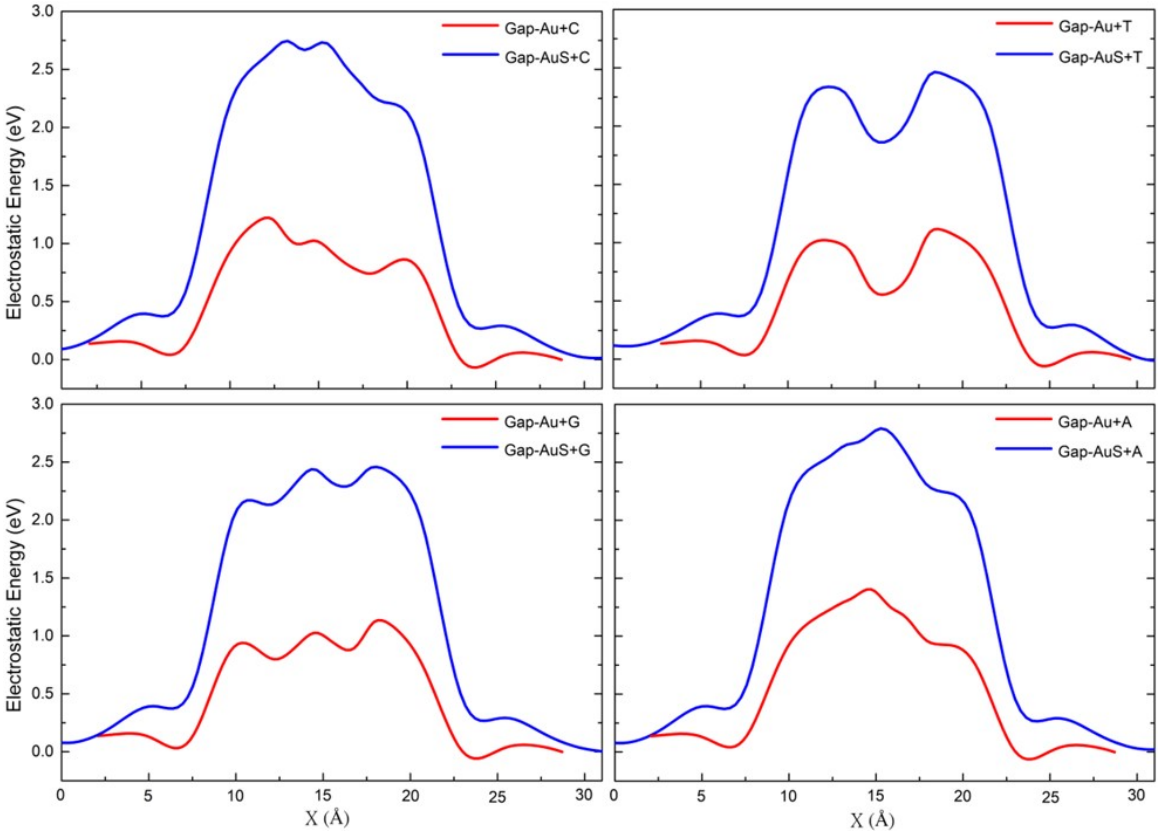

Fig S5. Electrostatic energy of Gap-Au (red line) and Gap-AuS (blue line), with each nucleobase in the nanogap.

Transmission and PDOS for different orientations

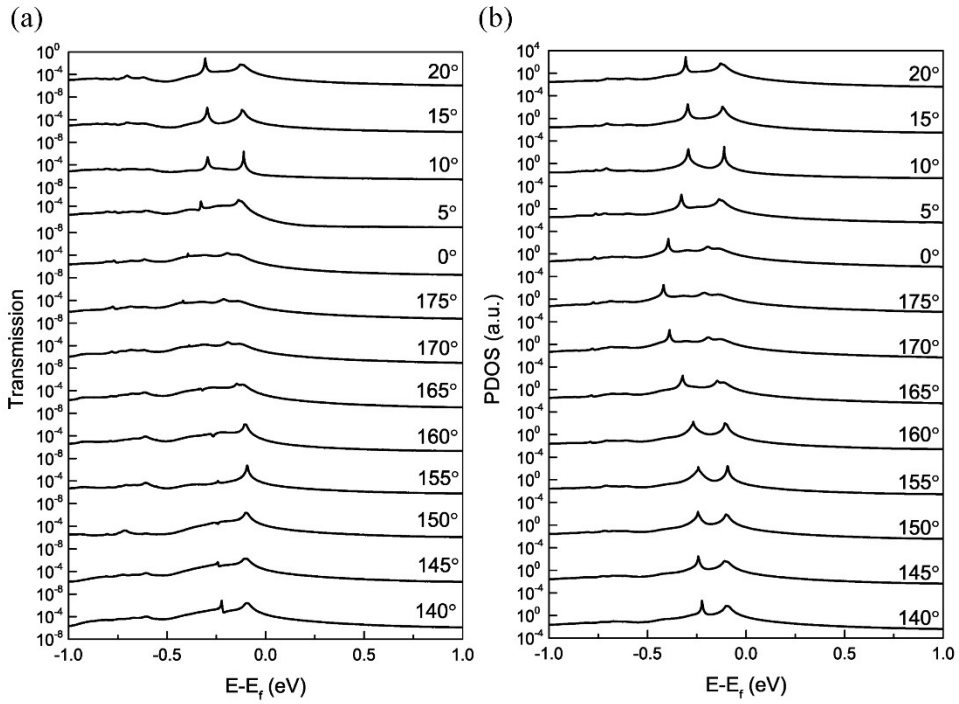

Fig S6. Transmission coefficients (a) and PDOS (b) of each orientation which contributes to average current for guanine in Gap-AuS. DOS of electrodes is excluded for clarity.

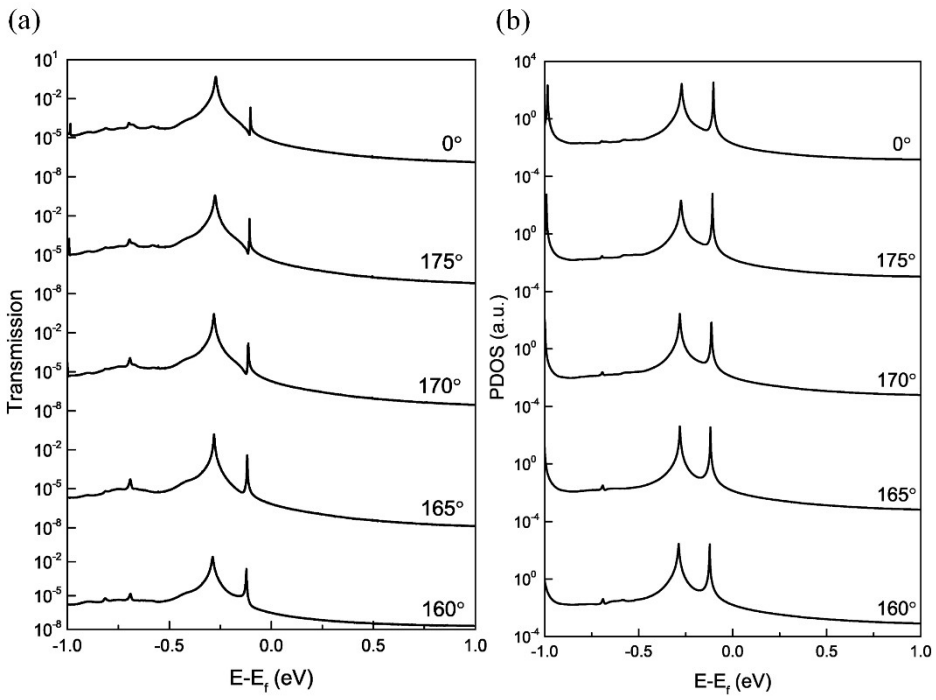

Fig S7. Transmission coefficients (a) and PDOS (b) of each orientation which contributes to average current for adenine in Gap-AuS. DOS of electrodes is excluded for clarity.

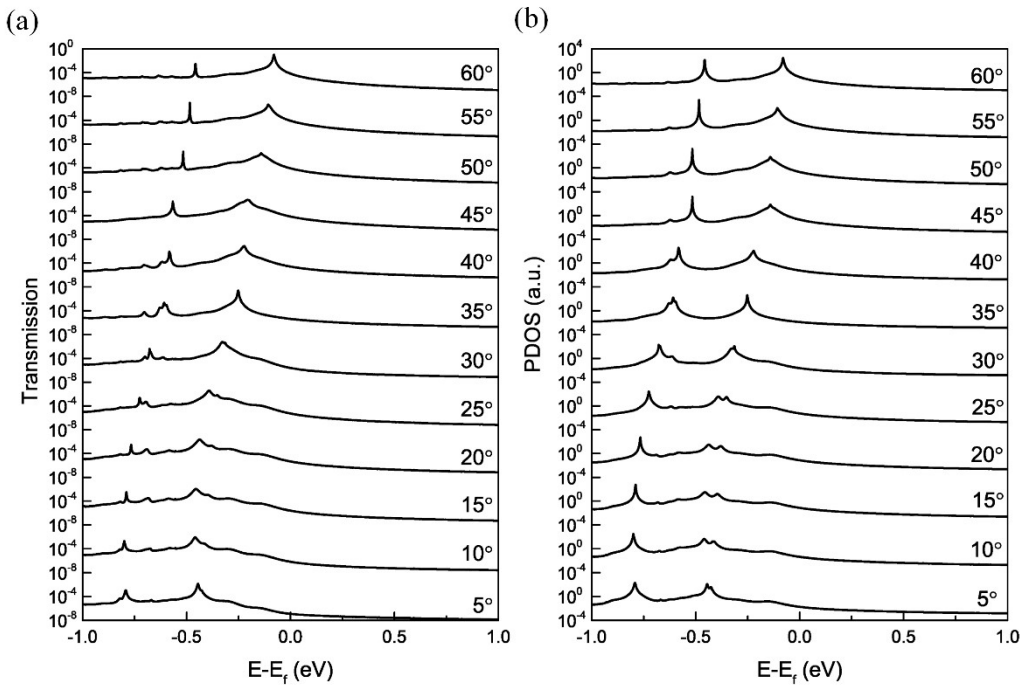

Fig S8. Transmission coefficients (a) and PDOS (b) of each orientation which contributes to average current for cytosine in Gap-AuS. DOS of electrodes is excluded for clarity.

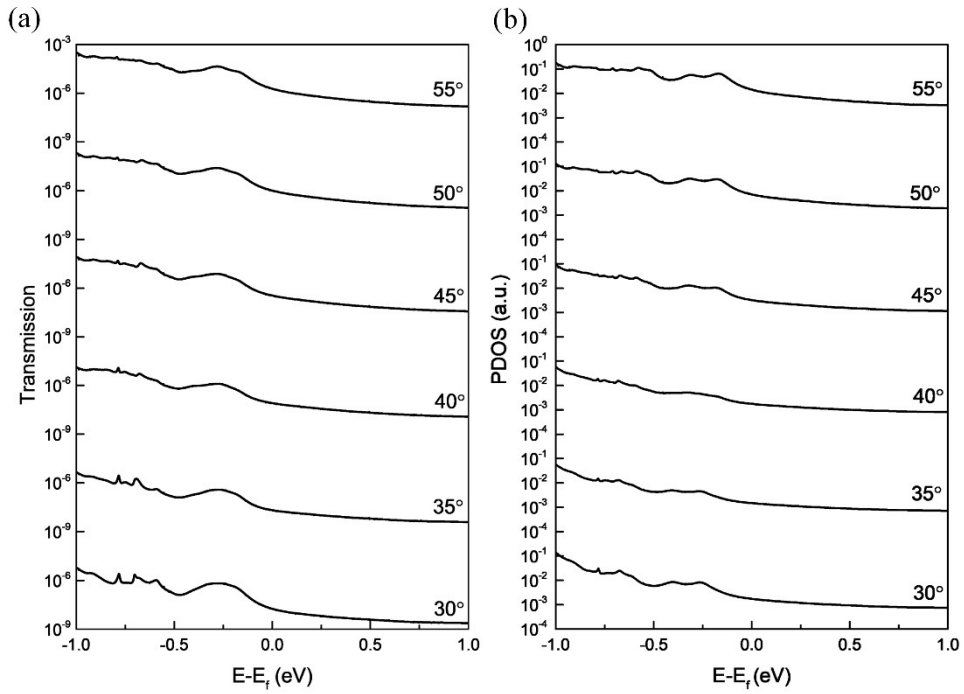

Fig S9. Transmission coefficients (a) and PDOS (b) of each orientation which contributes to average current for thymine in Gap-AuS. DOS of electrodes is excluded for clarity.

Table S2. Relative energy of nucleobases in Gap-Au at different orientations

Relative energy (eV)	Guanine	Adenine	Cytosine	Thymine
0°	0.107	0.215	0.111	0.198
5°	0.115	0.266	0.085	0.186
10°	0.100	0.264	0.064	0.167
15°	0.082	0.248	0.048	0.143
20°	0.080	0.215	0.033	0.115
25°	0.081	0.179	0.015	0.092
30°	0.064	0.143	0.000	0.066
35°	0.031	0.117	0.002	0.042
40°	0.000	0.117	0.028	0.017
45°	0.003	0.151	0.067	0.002
50°	0.075	0.202	0.119	0.000
55°	0.226	0.254	0.169	0.025
60°	0.452	0.300	0.211	0.087
65°	0.731	0.349	0.247	0.193
70°	1.040	0.349	0.274	0.331
75°	1.385	0.405	0.294	0.457
80°	1.753	0.462	0.307	0.532
85°	2.155	0.496	0.315	0.551
90°	2.553	0.498	0.318	0.547
95°	2.793	0.477	0.315	0.550
100°	2.733	0.441	0.309	0.542
105°	2.527	0.397	0.303	0.493
110°	2.401	0.346	0.295	0.400
115°	2.402	0.286	0.278	0.290
120°	2.387	0.217	0.265	0.204
125°	2.323	0.152	0.242	0.156
130°	1.968	0.098	0.216	0.141
135°	1.423	0.058	0.188	0.146
140°	0.961	0.025	0.161	0.159
145°	0.639	0.005	0.137	0.173
150°	0.409	0.000	0.121	0.182
155°	0.235	0.014	0.120	0.190
160°	0.111	0.039	0.114	0.192
165°	0.036	0.079	0.118	0.197
170°	0.008	0.120	0.133	0.202
175°	0.027	0.167	0.141	0.205
180°	0.091	0.210	0.134	0.201

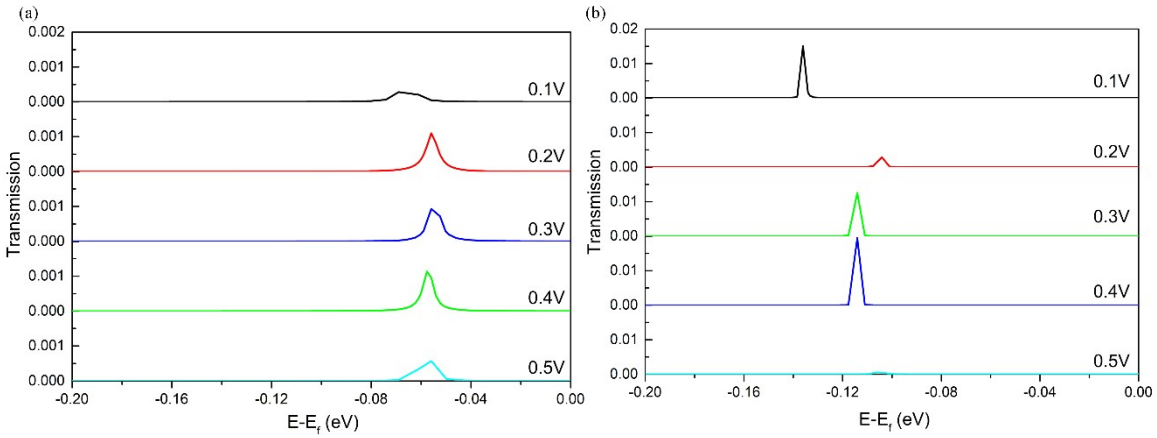

Fig. S10 Transmission of guanine-45° (a) and cytosine-5° (b) at different bias voltages within Gap-AuS'.

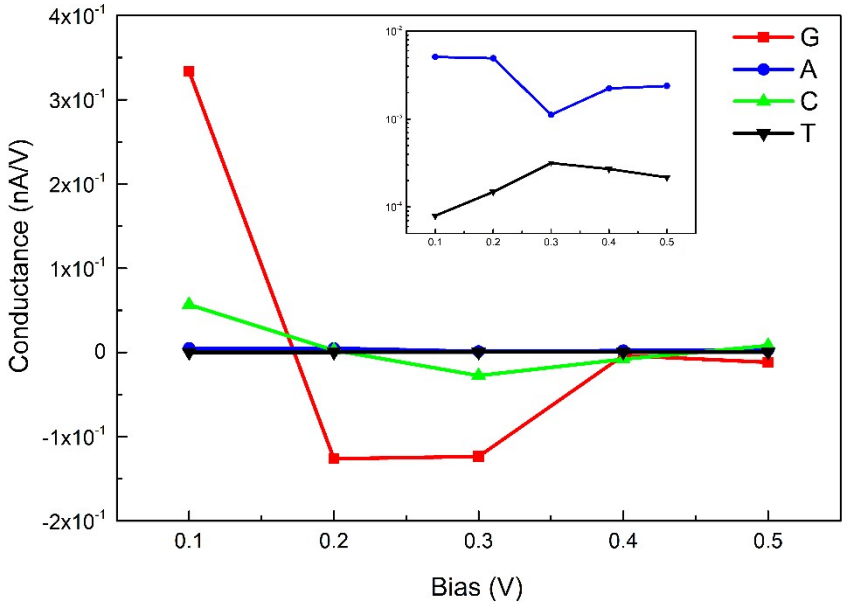

Fig. S11 Conductance-voltage curve for all the nucleobases in Gap-AuS'. Inset is the conductance-voltage curve plotted on a semilogarithmic scale for adenine and thymine.