Supplementary Information (SI) for Physical Chemistry Chemical Physics.

In-depth electronic behavior of pentagraphene and pentagonal-silicene sheets for DNA nucleic-base detection: implications for genetic biomarker sensing

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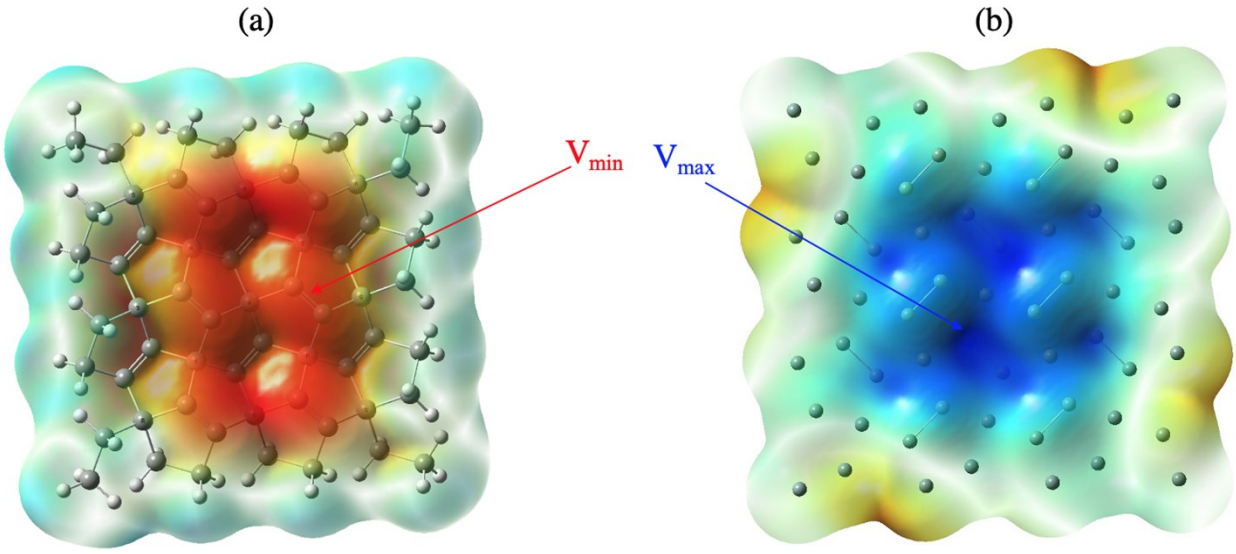

Fig. S1. MESP of the Substrates using the M062X/6-31G* level of theory (a) Penta graphene (b) Penta-silicene. Red arrow and blue arrow show the location of maximum negative potential and maximum positive potential.

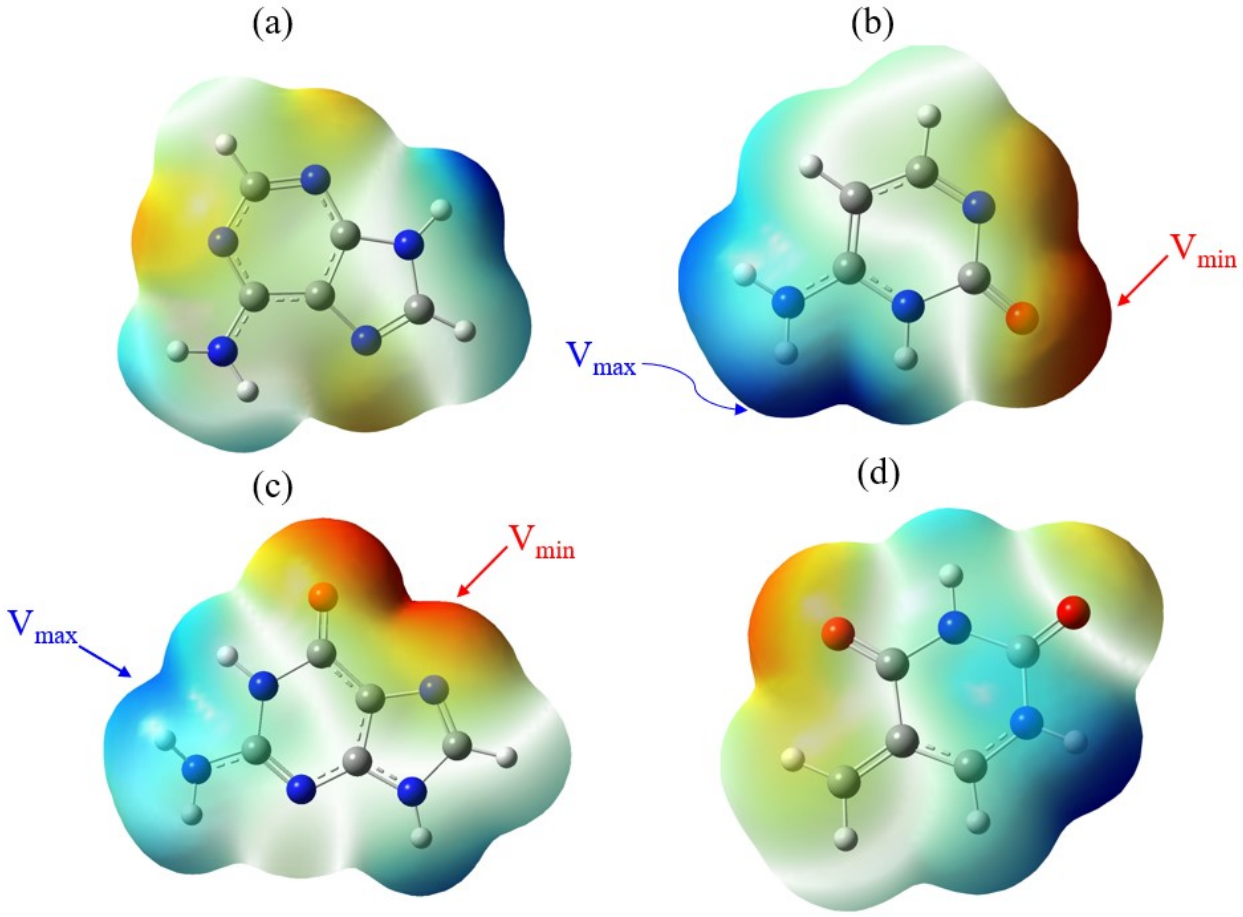

Fig S2. MESP of the DNA nucleic bases using the M062X/6-31G* level of theory (a)Adenine (b) Guanine (c) Cytosine and (d) Thymine. Red arrow and blue arrow show the location of minimum negative potential (V_{min}) and maximum positive potential (V_{max}).

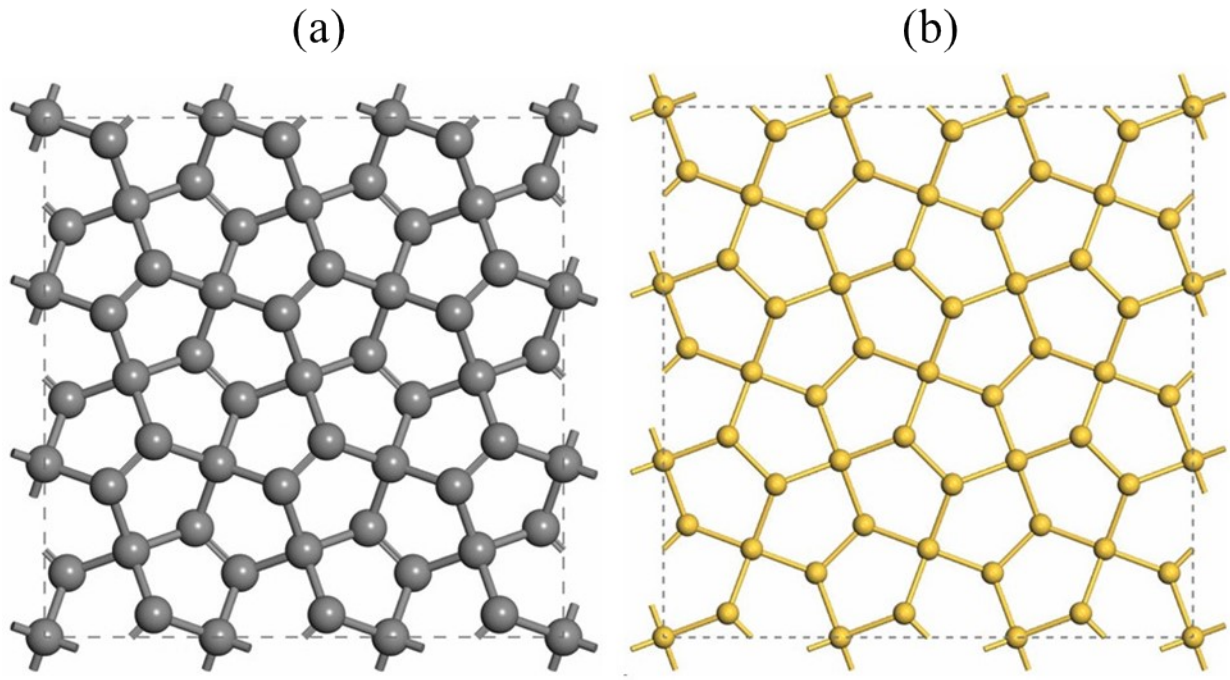

Fig S3. Optimized structures of (a) pentagraphene (PG) and (b) penta-silicene (p-Si). Grey sphere represent C atoms and yellow spheres represent Si atoms

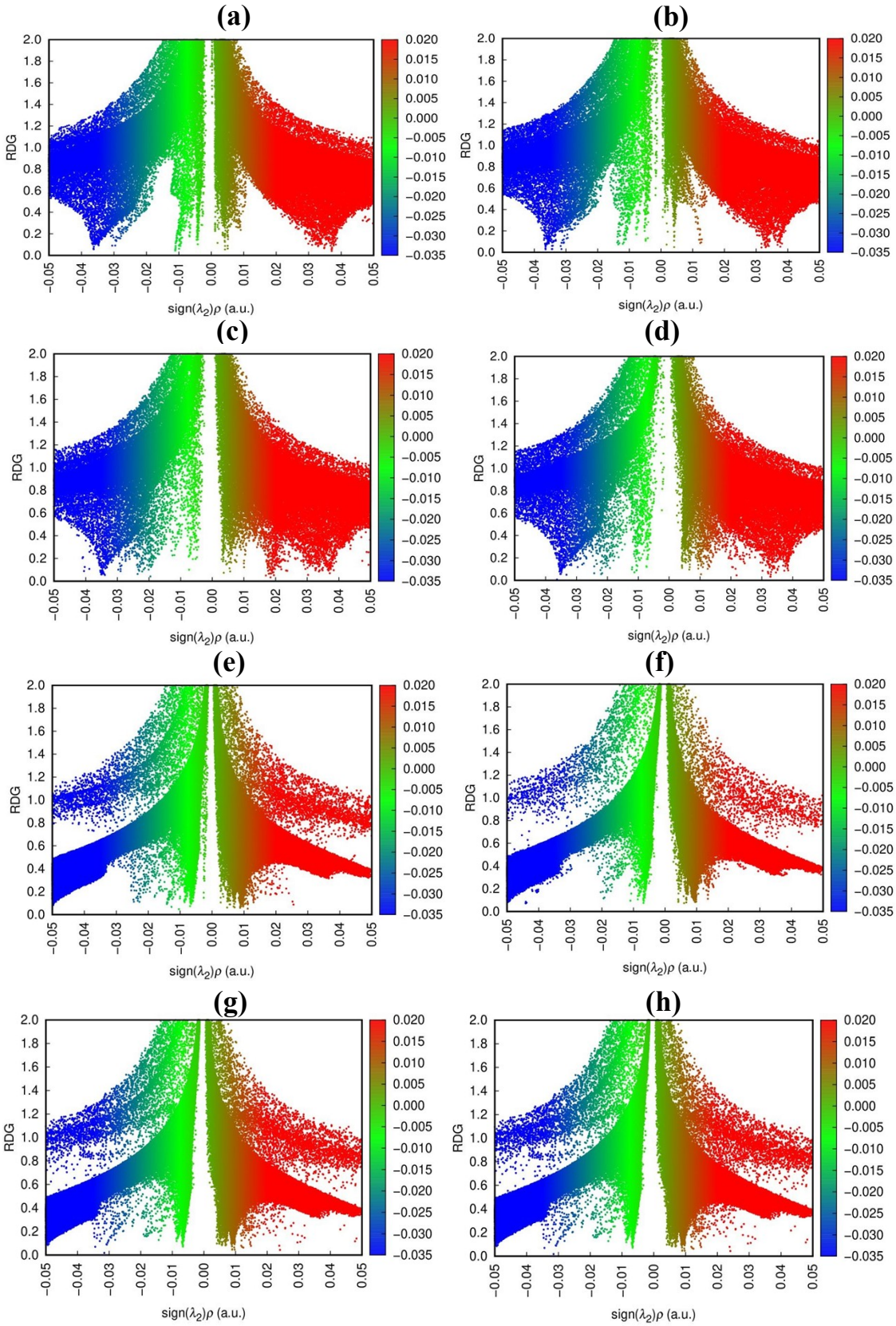
(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)
RDG
sign(λ2)ρ (a.u.)

Fig. S4. The RDG scatter diagrams of the PG-nucleic base complexes with (a) adenine (b) cytosine (c) guanine (d) thymine and p-Si-nucleic base complexes with (e) adenine (f) cytosine (g) guanine (h) thymine. The iso-surfaces are colored according to the values of 0.5 a.u respectively.

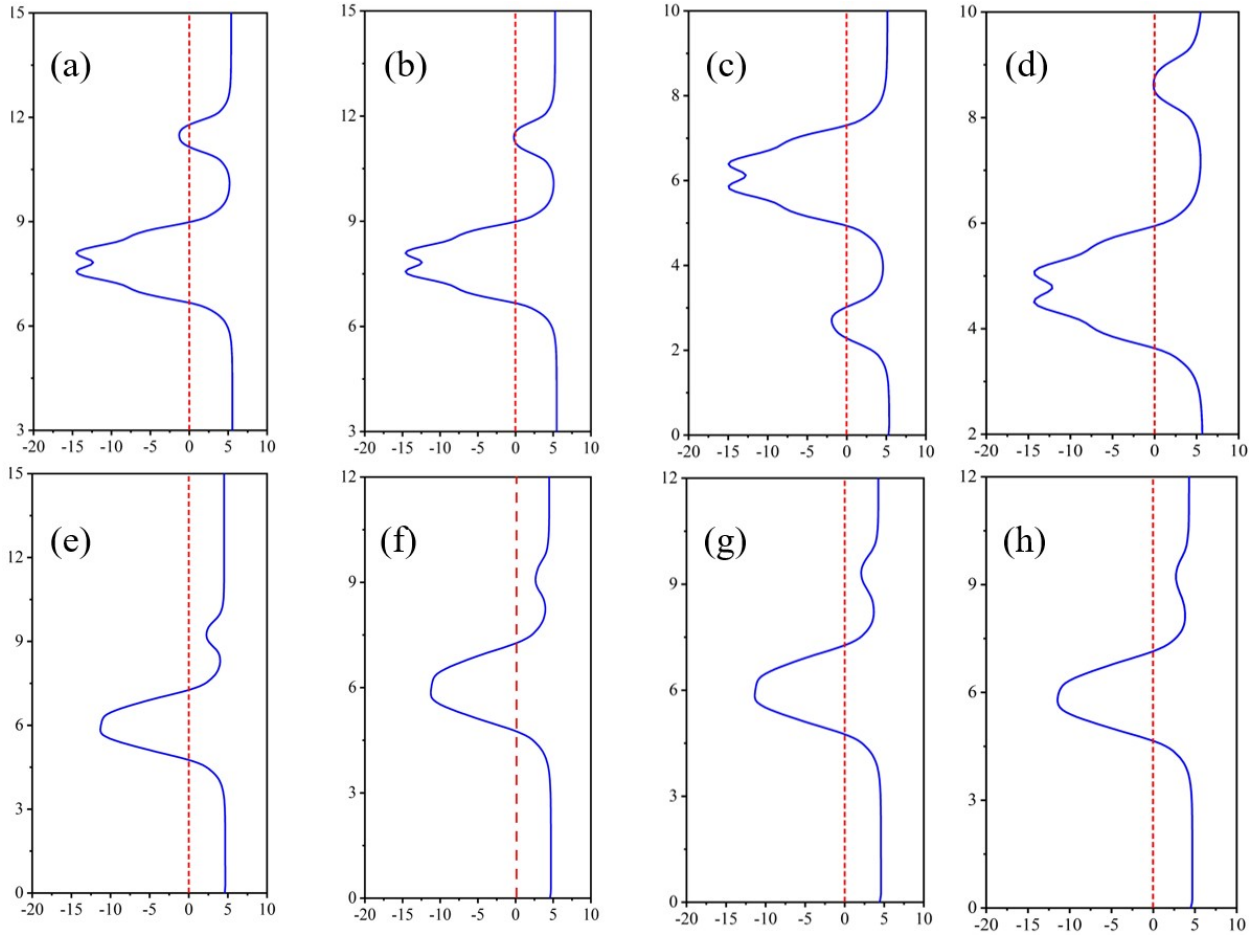

Fig. S5. Calculated electrostatic potential of the PG-nucleic base complexes with (a) adenine (b) cytosine (c) guanine (d) thymine and p-Si-nucleic base complexes with (e) adenine (f) cytosine (g) guanine (h) thymine.

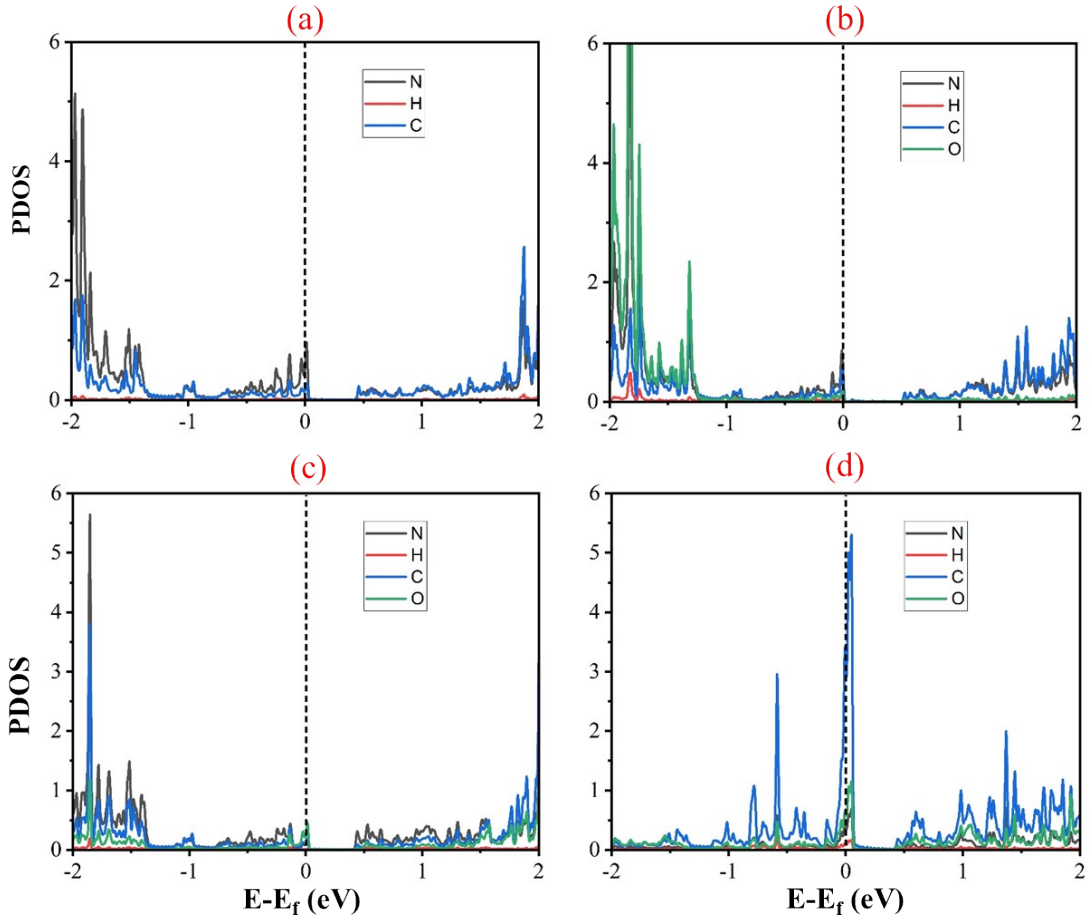

Figure S6. PDOS of (a) p-Si-Adenine (b) p-Si-Cytosine (c) p-Si-Guanine and (d) p-Si-Thymine.

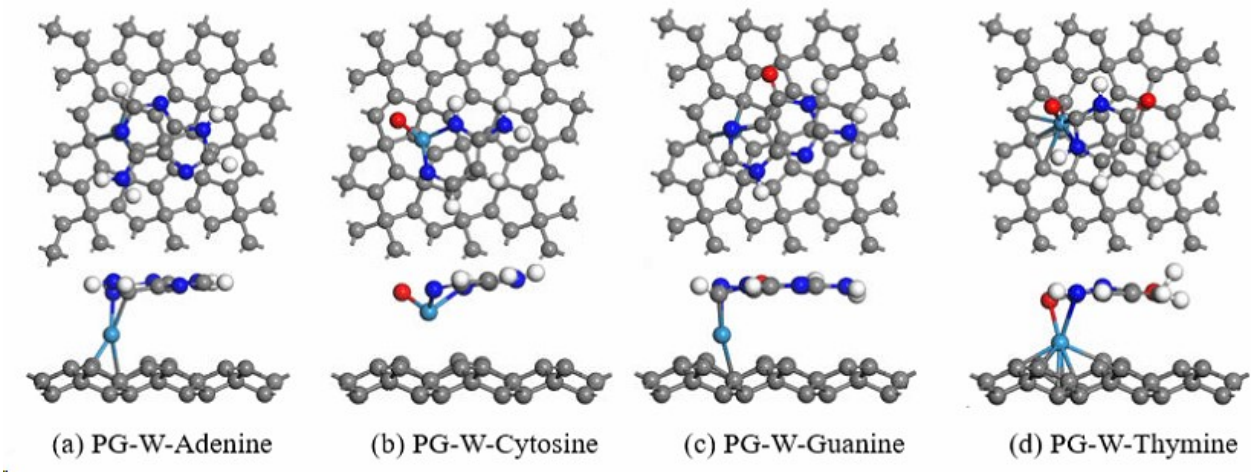

Fig. S7. Top and side views of the optimized configurations of single nucleobases (a: Adenine; b: Guanine; c: Cytosine; d: Thymine) on Tungsten (W) doped PG sheet. (gray sphere is C atom; white sphere is H atom; red sphere is O atom; blue sphere is N atom; Yellow sphere is Au atom).

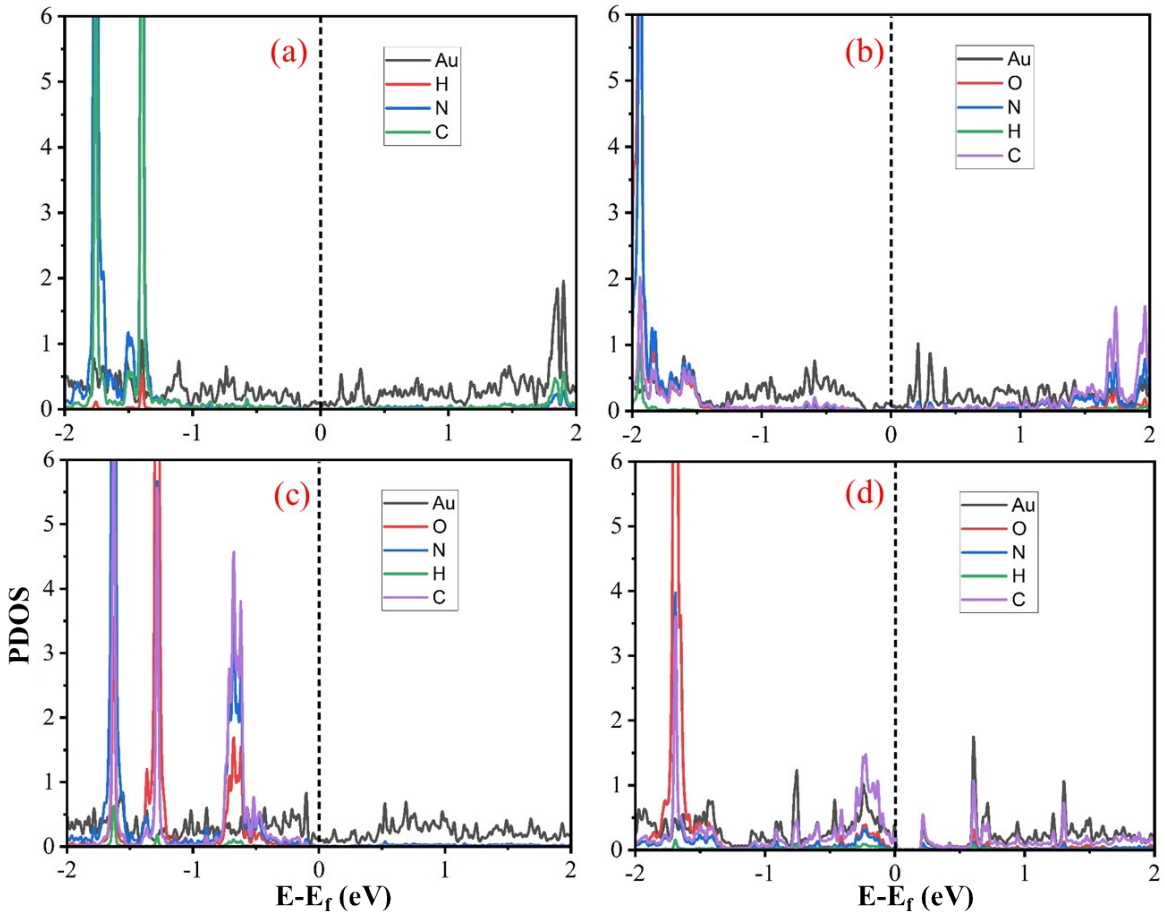

Figure S8. PDOS of (a) p-Si-Au-Adenine (b) p-Si-Au-Cytosine (c) p-Si-Au-Guanine and (d) p-Si-Au-Thymine.

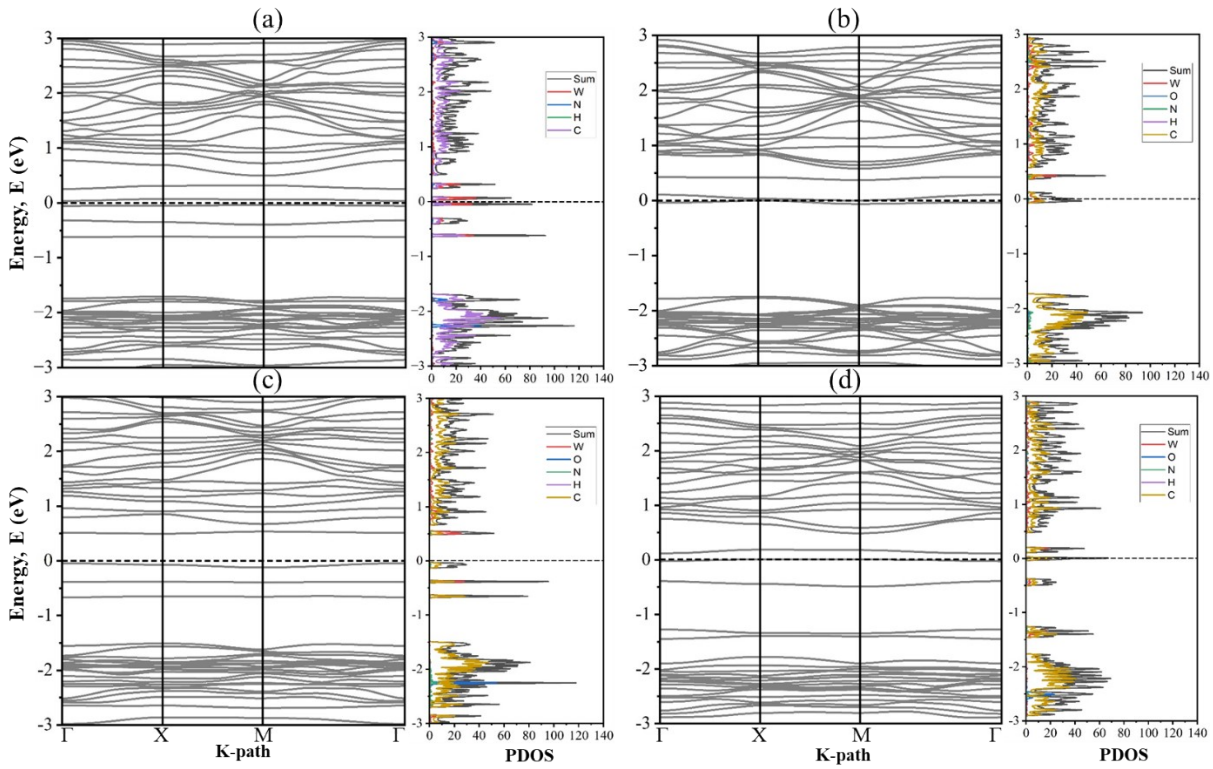

Fig. S9. Total electronic band structure and PDOS of (a) PG-W-Adenine (b) PG-W-Cytosine (c) PG-W-Guanine and (d) PG-W-Thymine

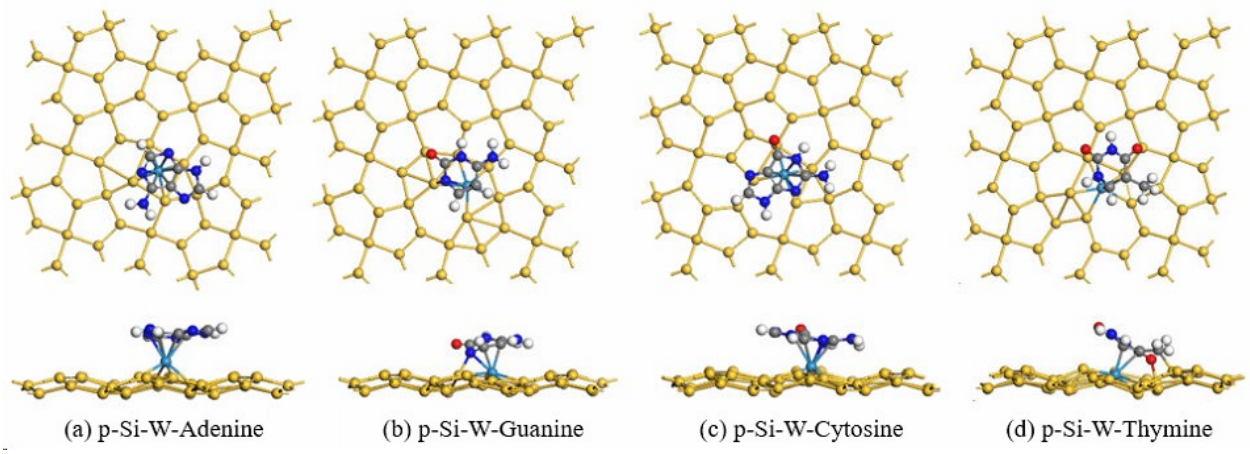

Fig. S10. Top and side views of the optimized configurations of single nucleobases (a: Adenine; b: Guanine; c: Cytosine; d: Thymine) on W dopped p-Si sheet. (Yellow sphere is Si atom; white sphere is H atom; red sphere is O atom; blue sphere is N atom; cyan sphere is W atom).

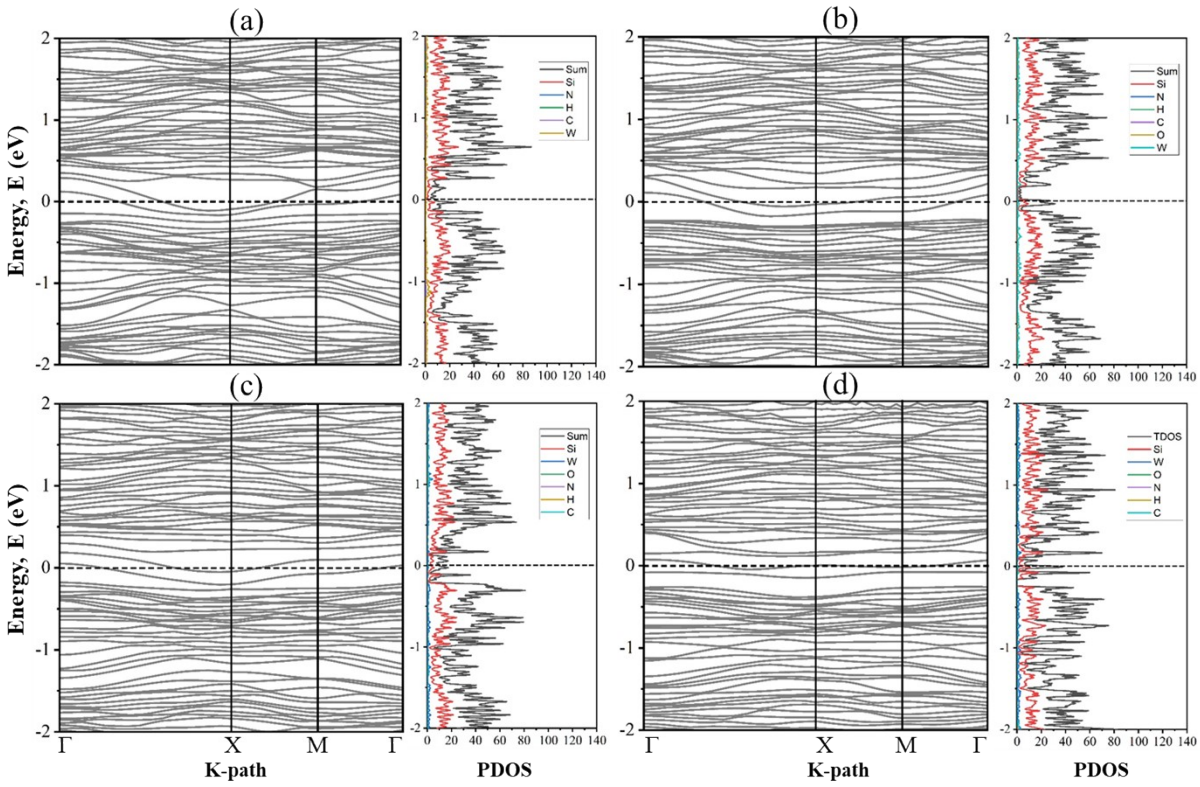

Fig. S11. Total electronic band structure and PDOS of (a) p-Si-W-Adenine (b) p-Si-W-Cytosine (c) p-Si-W-Guanine and (d) p-Si-W-Thymine.

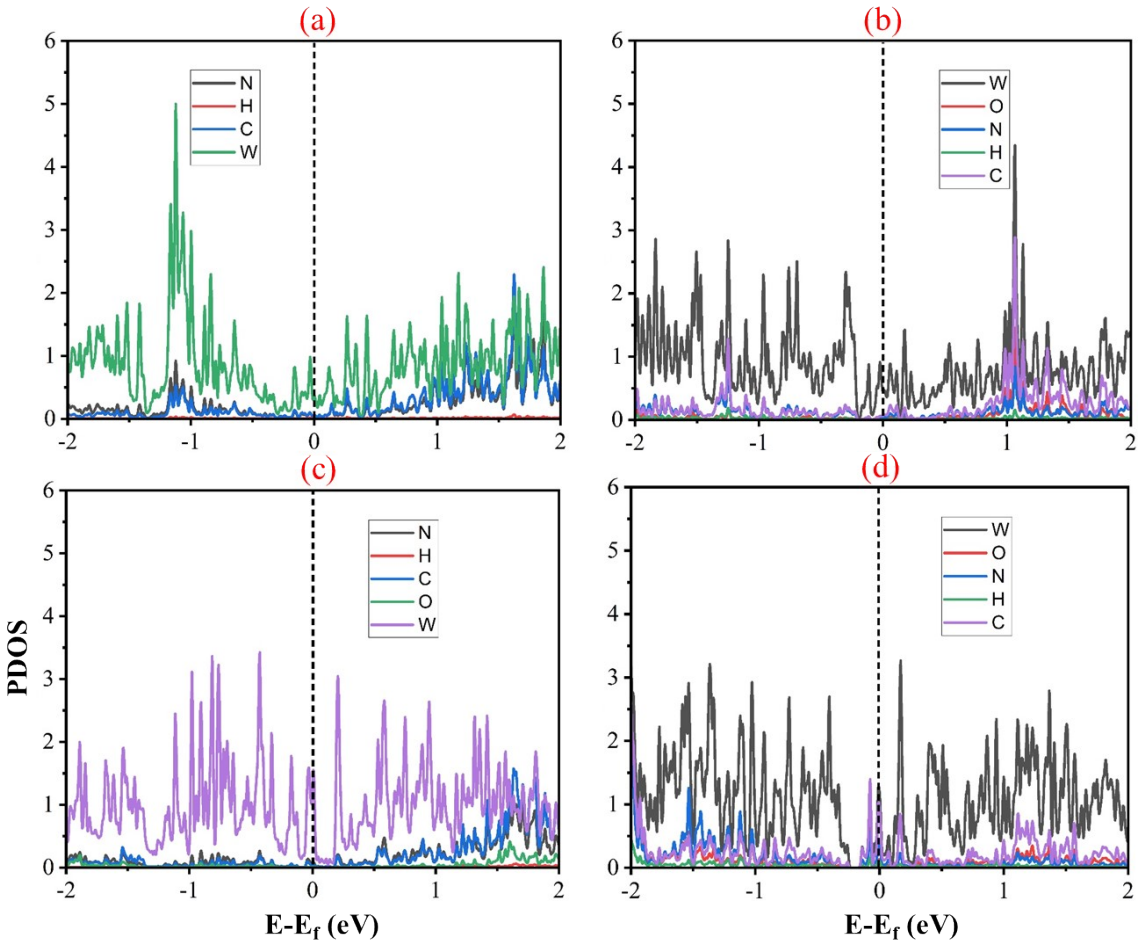

Figure S12. PDOS of (a) p-Si-W-Adenine (b) p-Si-W-Cytosine (c) p-Si-W-Guanine and (d) p-Si-W-Thymine.

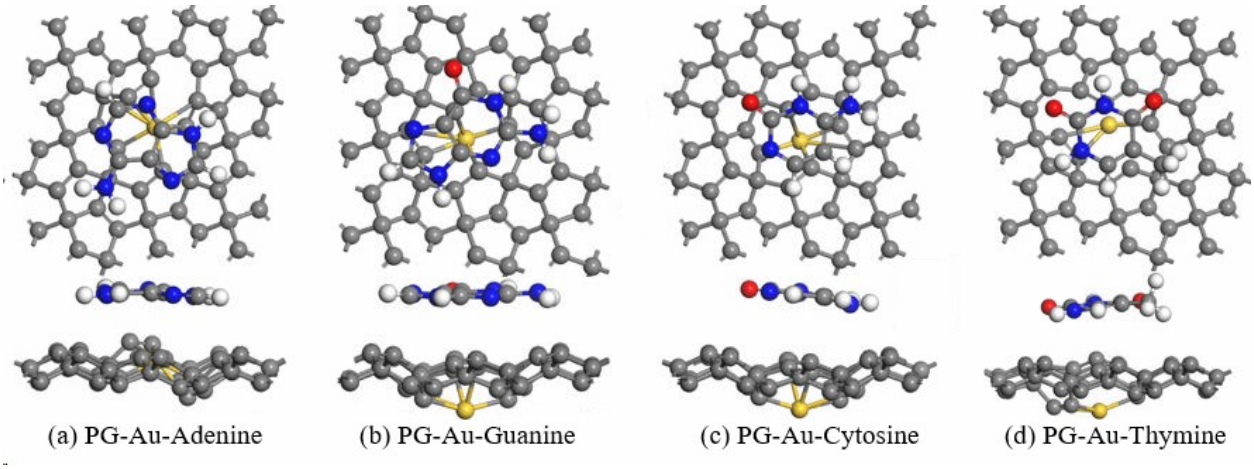

Fig. S13. Top and side views of the optimized configurations of single nucleobases (a: Adenine; b: Guanine; c: Cytosine; d: Thymine) on Tungsten (Au) functionalized PG sheet. (gray sphere is C atom; white sphere is H atom; red sphere is O atom; blue sphere is N atom; yellow sphere is Au atom).

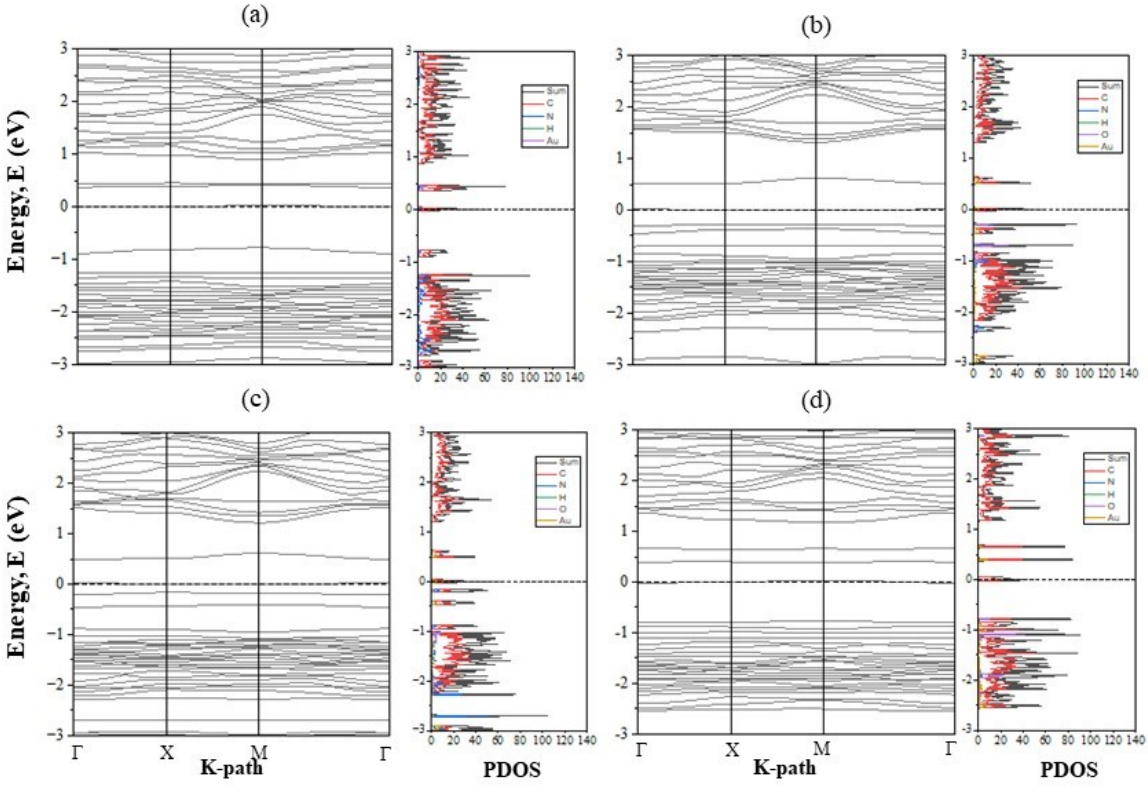

Fig. S14. Total electronic band structure and PDOS of (a) PG-Au-Adenine (b) PG-Au-Guanine (c) PG-Au-Cytosine and (d) PG-Au-Thymine.

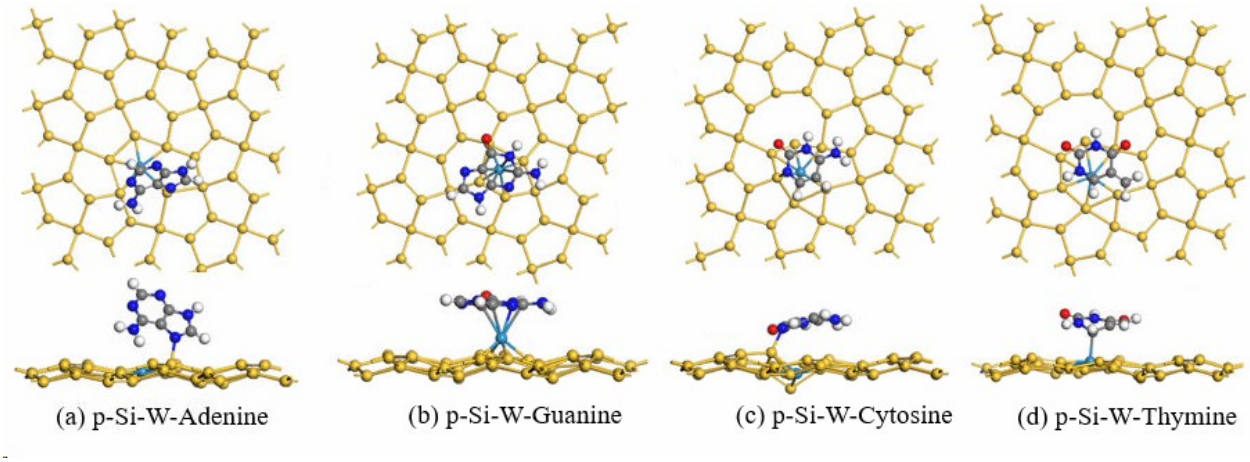

Fig. S15. Top and side views of the optimized configurations of single nucleobases (a: Adenine; b: Guanine; c: Cytosine; d: Thymine) on Tungsten (W) functionalized p-Si sheet. (gray sphere is C atom; white sphere is H atom; red sphere is O atom; blue sphere is N atom; teal sphere is W atom).

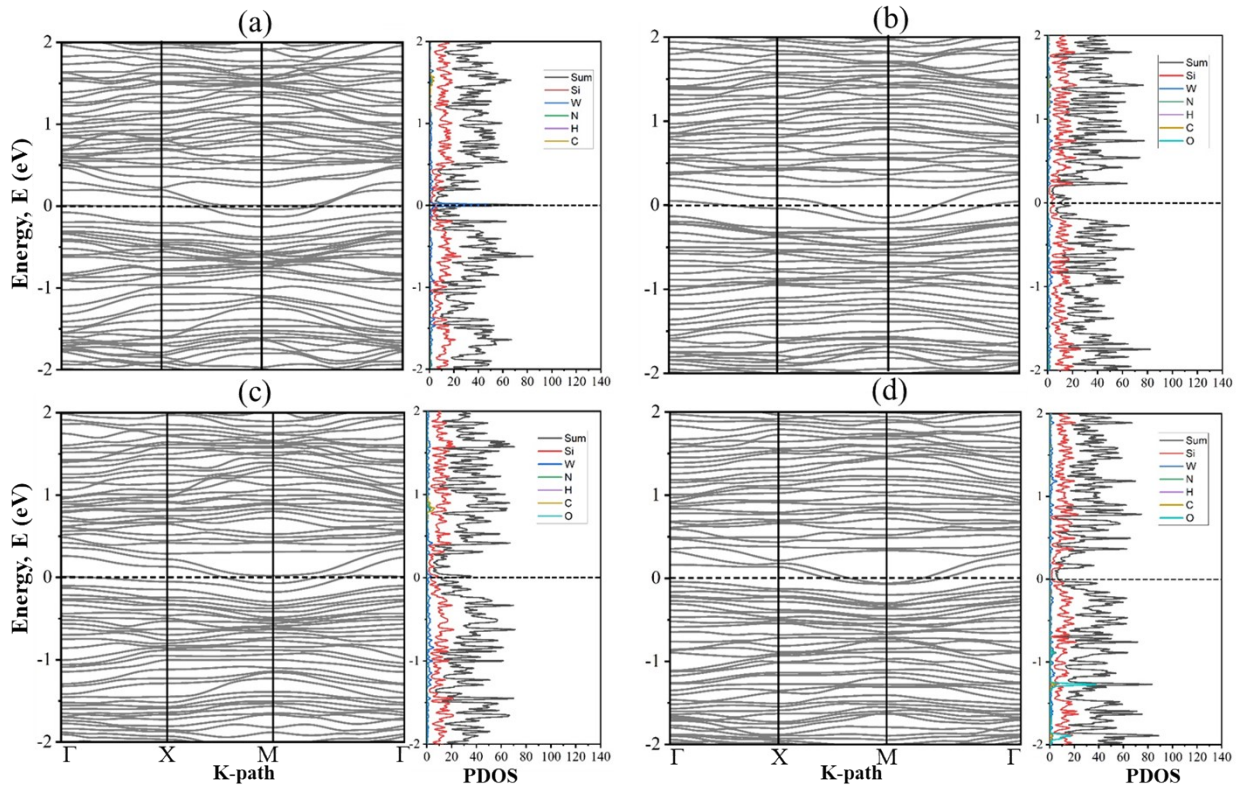

Fig. S16. Total electronic band structure and PDOS of (a) p-Si-W-Adenine (b) p-Si-W-Cytosine (c) p-Si-W-Guanine (d) p-Si-W-Thymine.