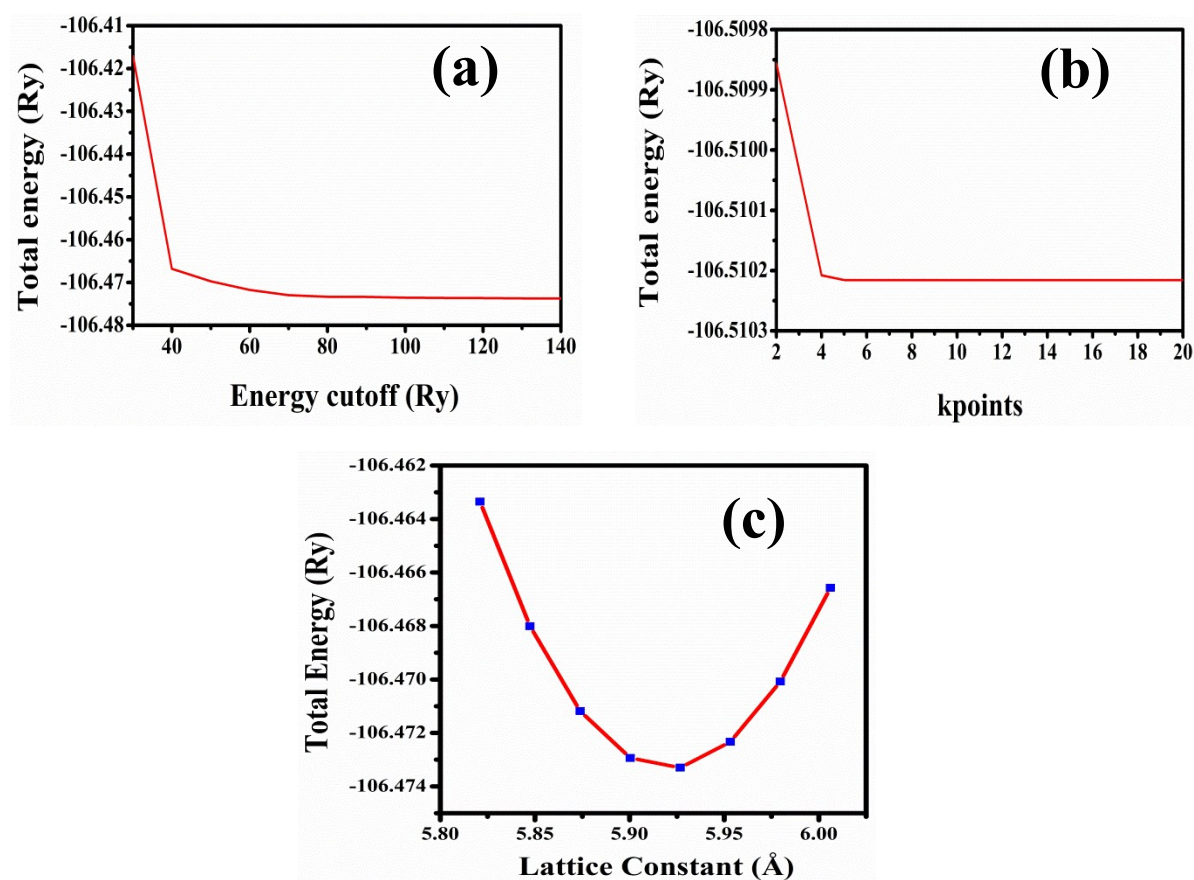


# “Haeckelite” a new low dimensional cousin of boron nitride for Biosensing with ultra-fast recovery time: A first principles investigation

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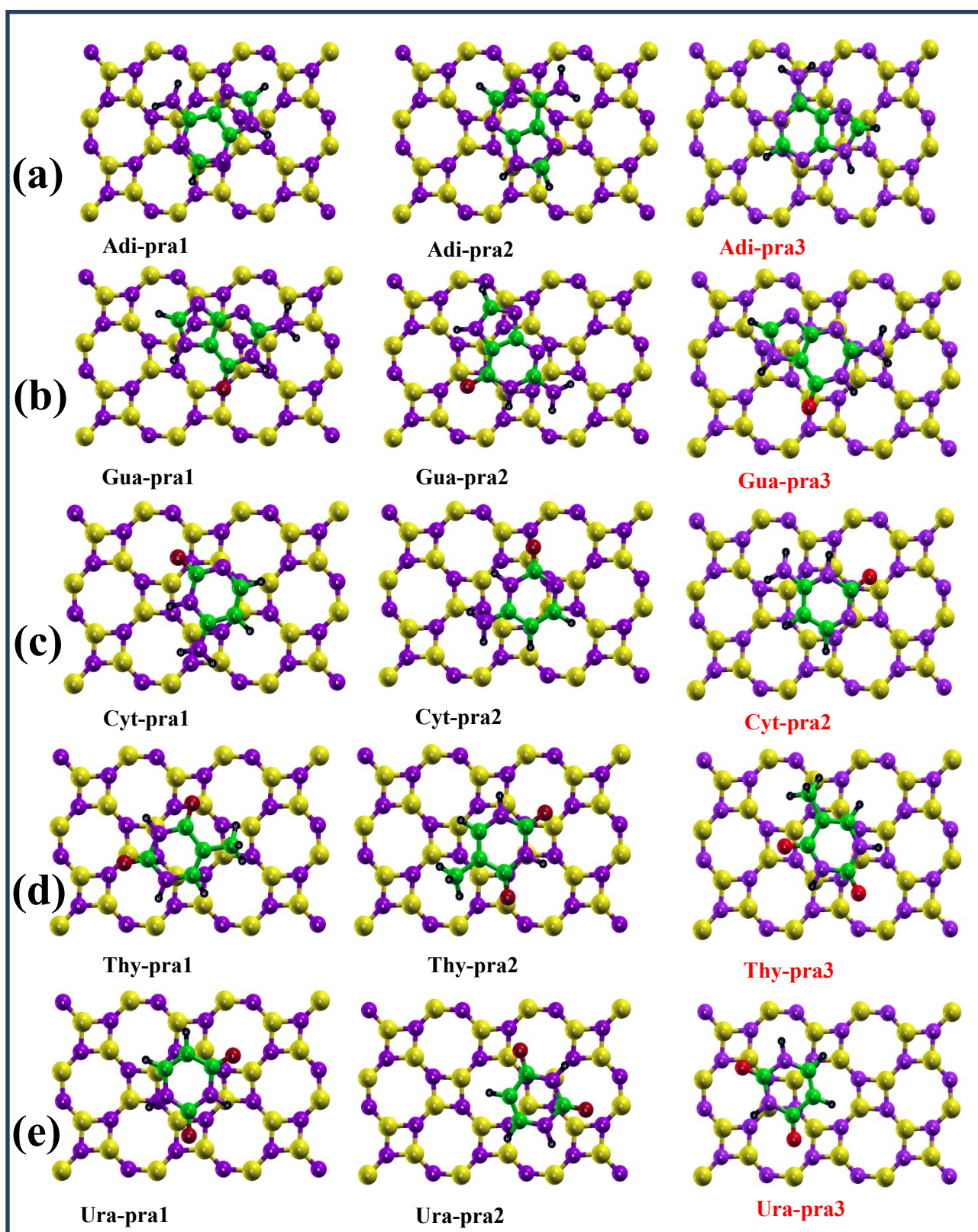
**Figure S1:** Total energy Convergence plot for haeck-BN (a) Energy cutoff (ecut), (b) K-point and (c) Energy of states (eos).

**Table S1:** Calculated total energy of nucleobase adsorbed heck-BN system. Red color represents minimum energy.

Distance (Å)	A	G	C	T	U
1.0	-797.14563569	-827.24450277	-778.32027206	-790.40151271	-793.01554085
1.5	-803.32734246	-835.14560366	-784.52685720	-801.55327009	-797.48784613
2.0	-805.07205702	-837.96243467	-786.28344130	-811.496918992	-798.86362140
2.5	-805.59573819	-839.04827443	-786.89557762	-813.26327259	-799.29076560
<b>Optimized</b>	<b>-805.70177593</b>	<b>-839.39961317</b>	<b>-787.04842003</b>	<b>-813.72913714</b>	<b>-799.37783694</b>
3.0	-805.69647630	-839.38631967	-787.03703933	-813.71807435	-799.39073438
3.5	-805.69071475	-839.38548052	-787.03216000	-813.71031933	-799.36672226
4.0	-805.67720738	-839.37047296	-787.02507247	-813.65860629	-799.35612839

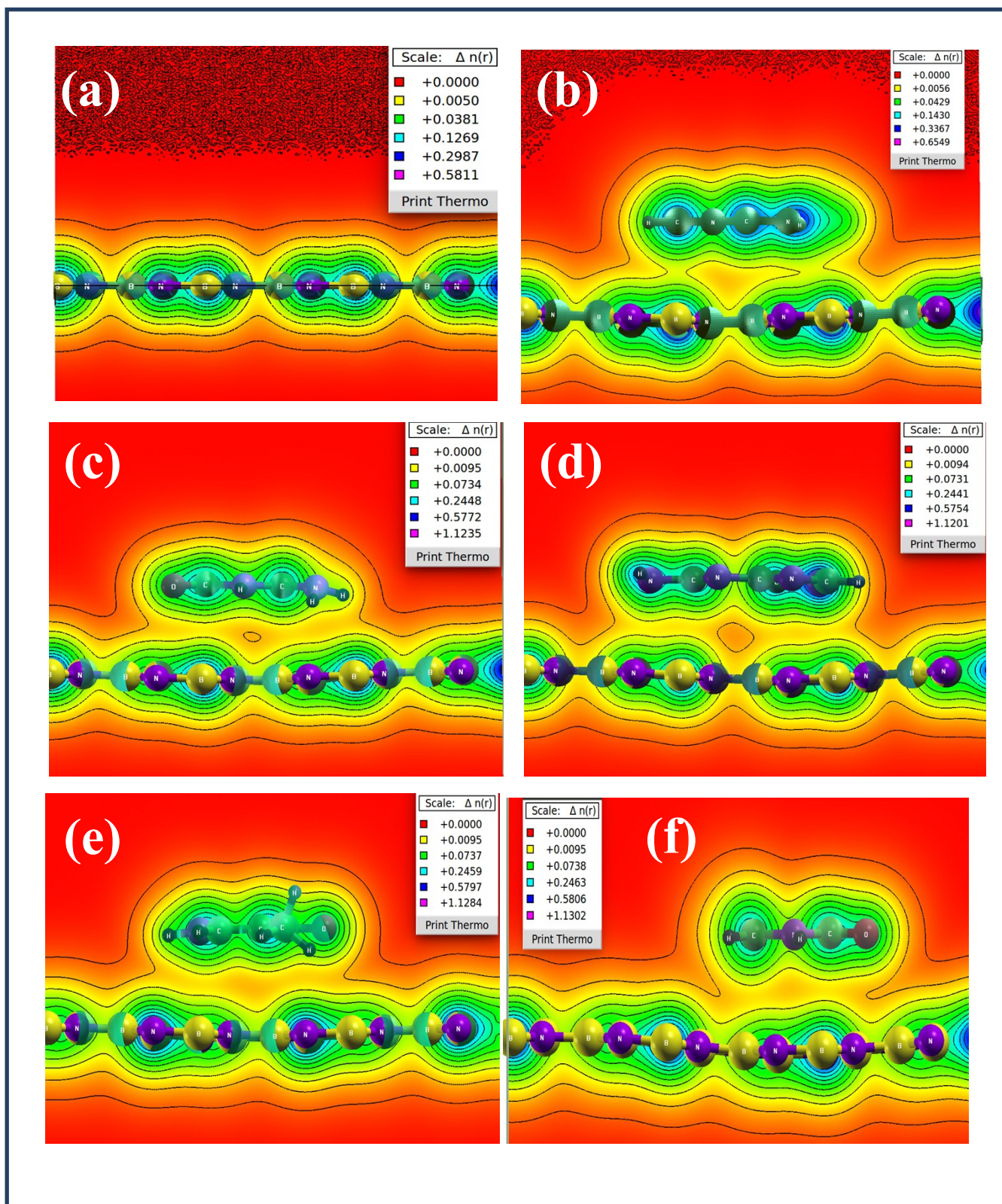
**Table S2:** Calculated total energy of nucleobase adsorbed heck-BN system with different orientation. Red color represents minimum energy.

System	Orientation			
	Perpendicular	Parallel		
		Parallel (1)	Parallel (2)	Parallel (3)
<b>A</b>	-805.67409951	-805.69333844	-805.70168216	<b>-805.70177593</b>
<b>G</b>	-839.36709371	-839.37120249	-839.39640827	<b>-839.39961217</b>
<b>C</b>	-787.02532204	-787.03926981	-787.04579516	<b>-787.04842003</b>
<b>T</b>	-813.63395282	-813.72114341	-813.72384597	<b>-813.72913714</b>
<b>U</b>	-799.35689170	-798.91355371	-798.85654916	<b>-799.37783694</b>

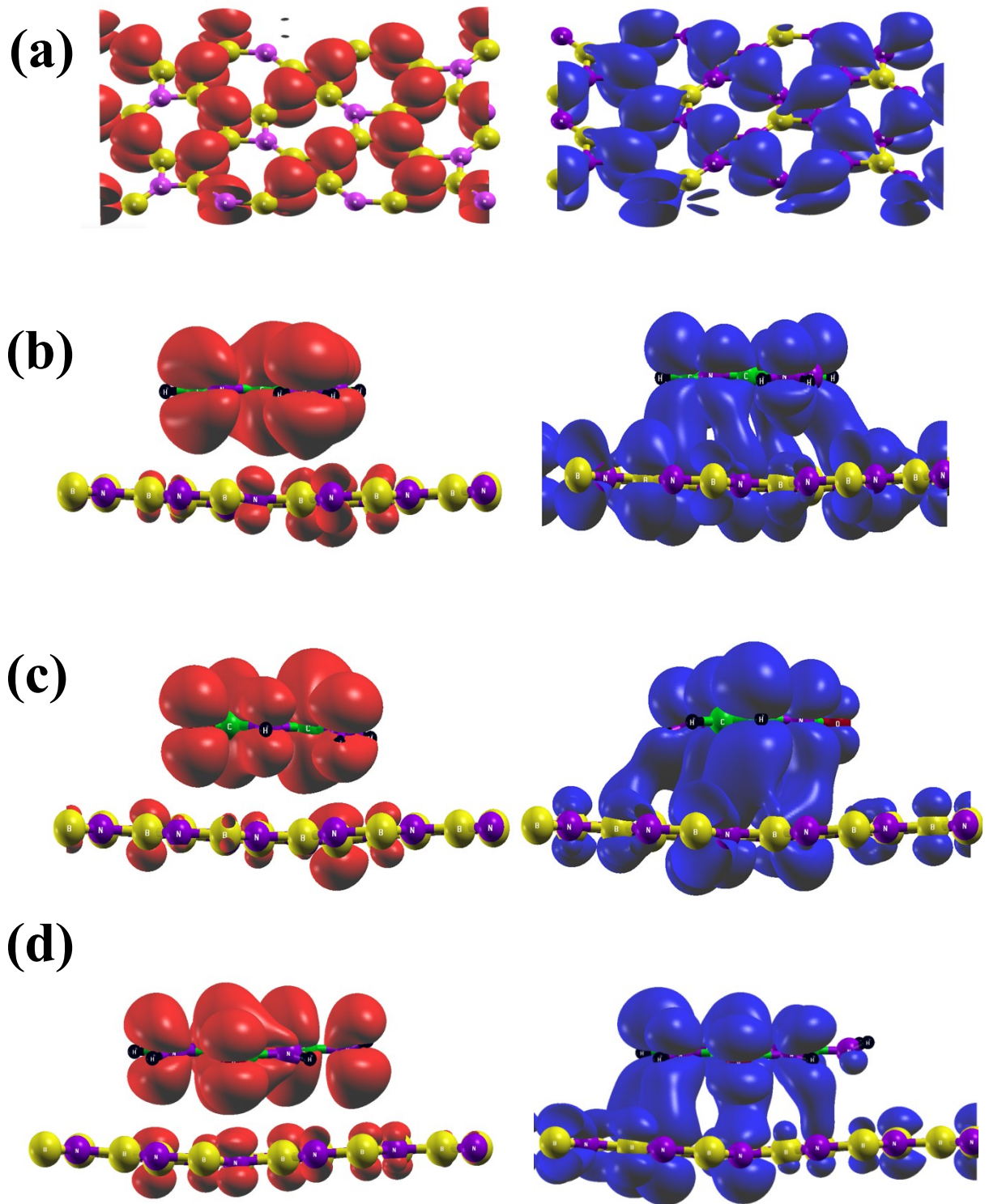


**Fig.S2.** Different parallel orientation of haeck-BN adsorbed by nucleobases (a) Adenine, (b) Cytosine, (c) Guanine, (d) Thymine, (e) Uracil.

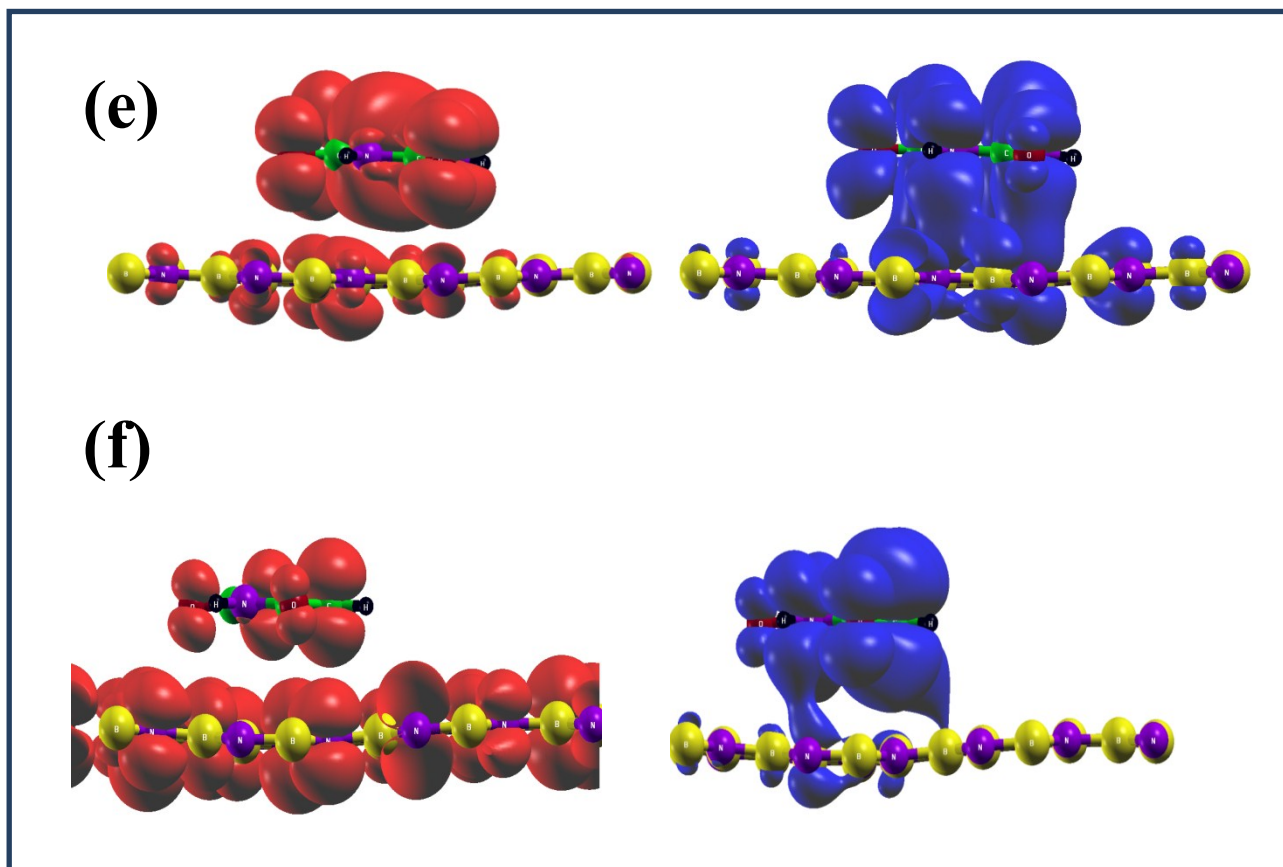




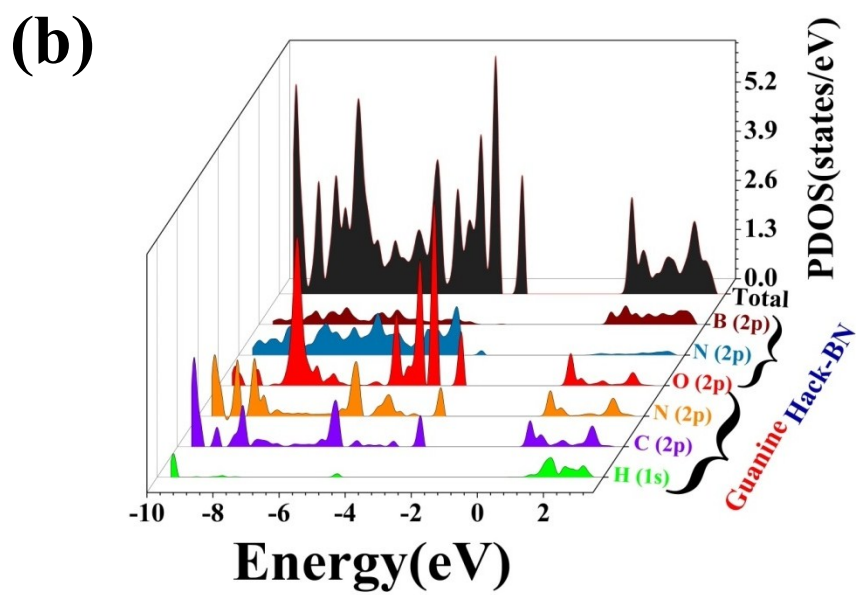
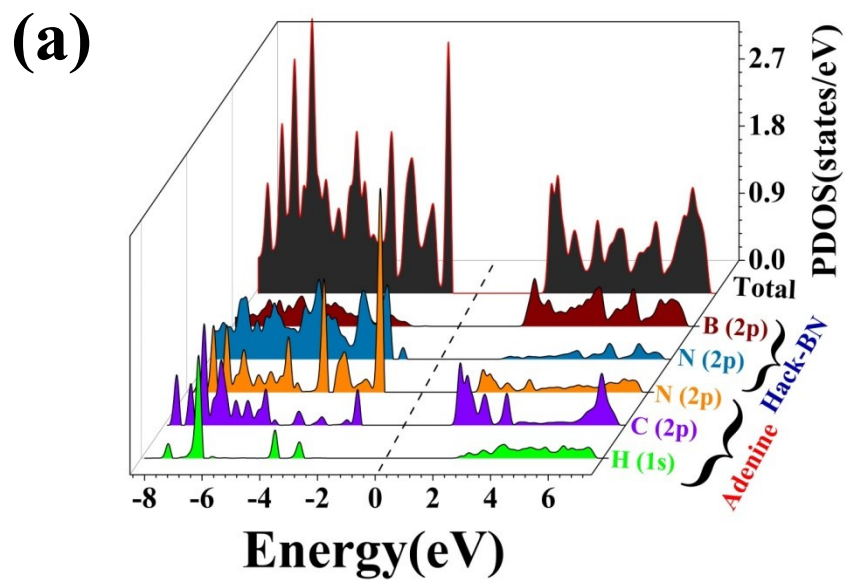
**Fig.S3.** Charge density plot of (a) haeck-BN and haeck-BN adsorb by nucleobases (b) Adenine, (c) Cytosine, (d) Guanine, (e) Thymine, (f) Uracil.





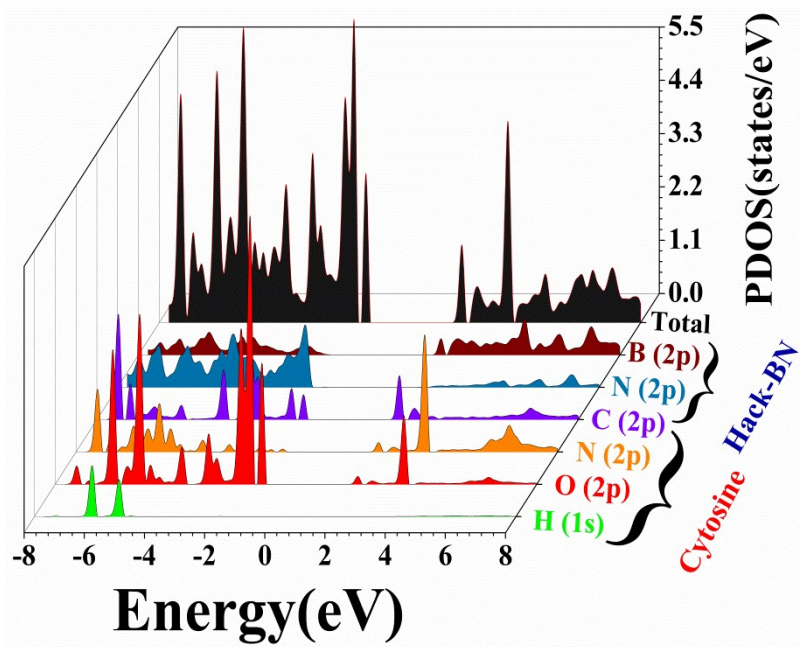


**Fig.S4.** HOMO and LUMO of (a) haeck-BN and (b-f) nucleobase adsorbed haeck-BN system; (b) Adenine, (c) Cytosine, (d) Guanine, (e) Thymine, (f) Uracil.

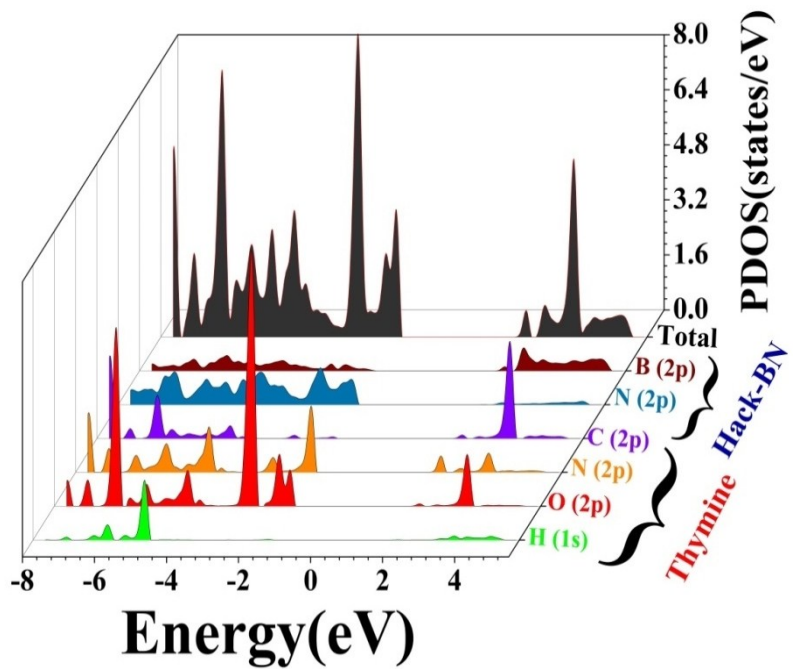




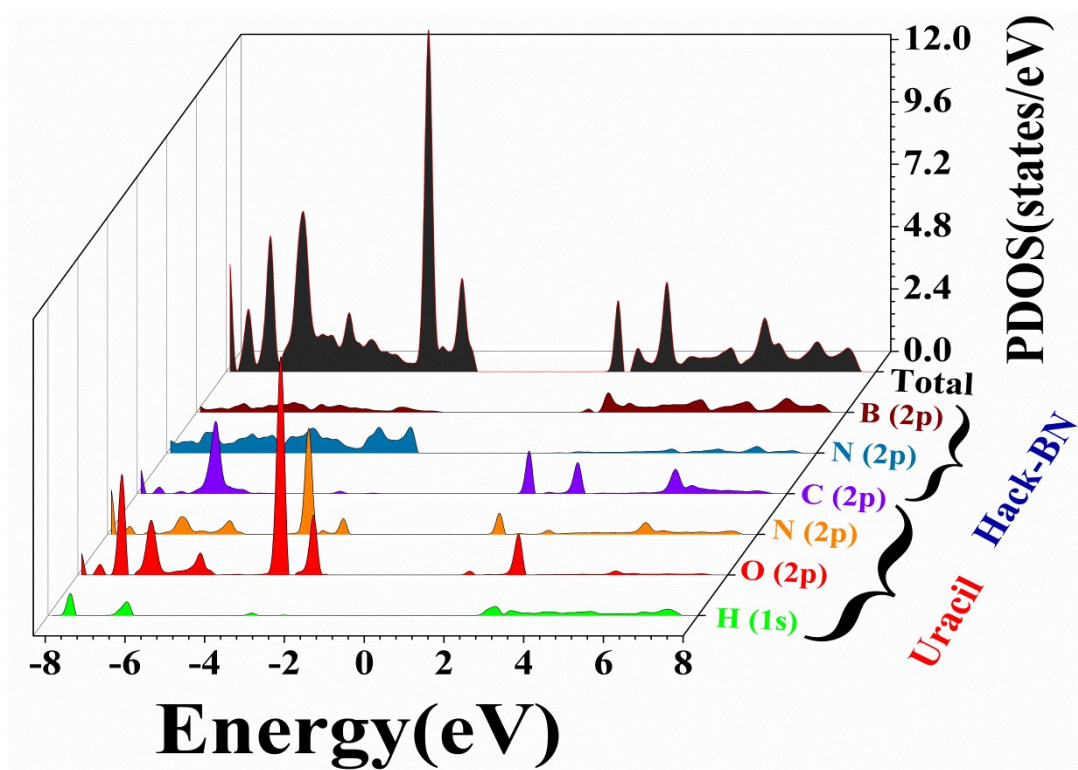
(c)



(d)

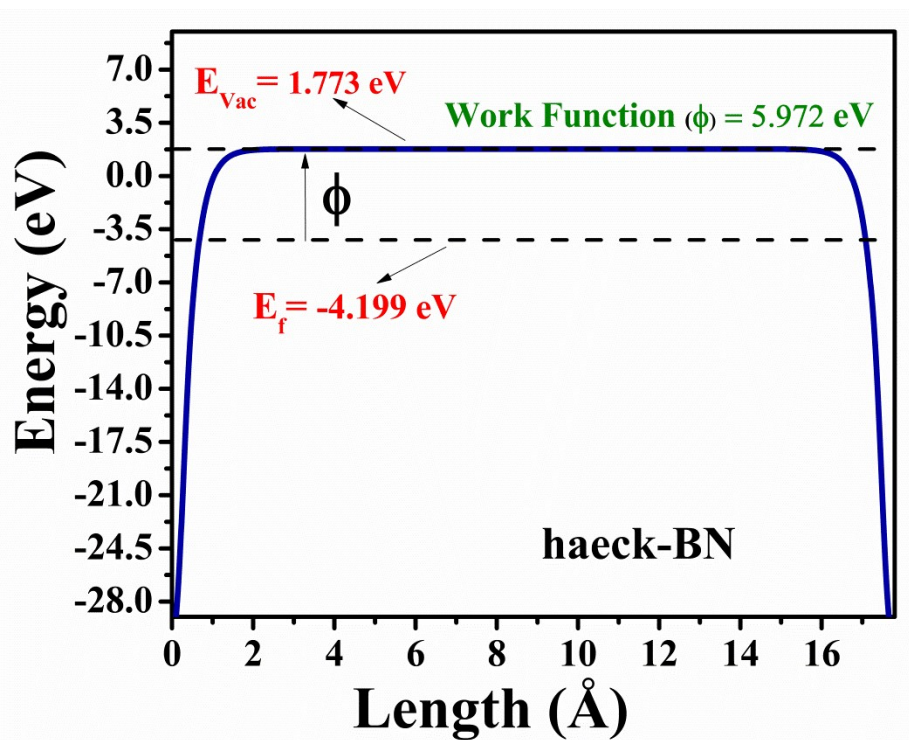


(e)

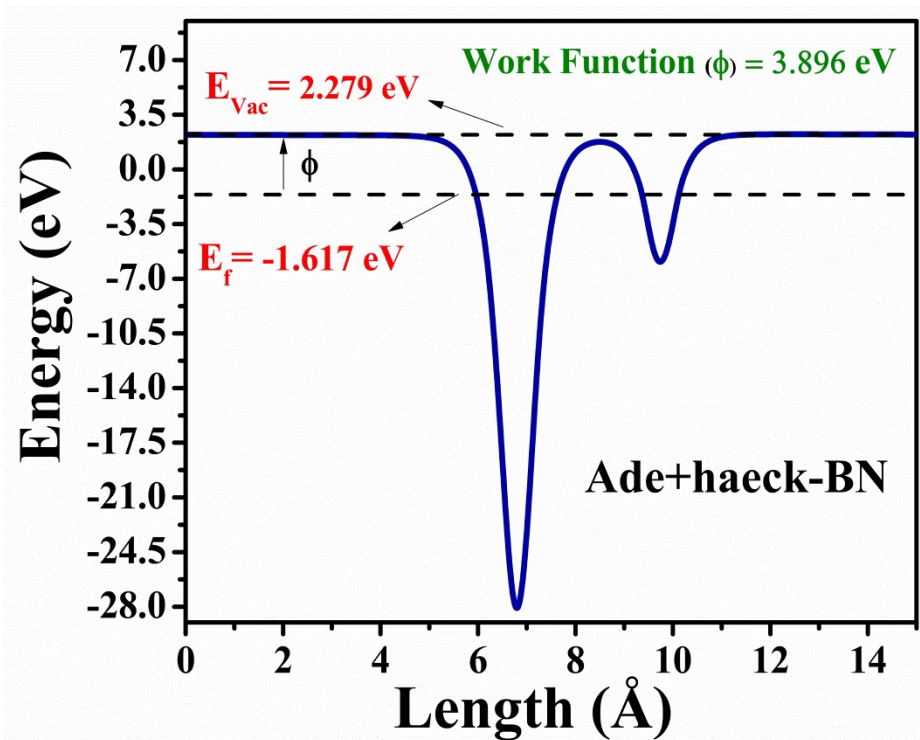


**Figure S5:** Partial density of states (PDOS) plot of nucleobases adsorbed haecK-BN system (a) Adenine, (b) Guanine, (c) Cytosine, (d) Thymine and (e) Uracil.

(a)

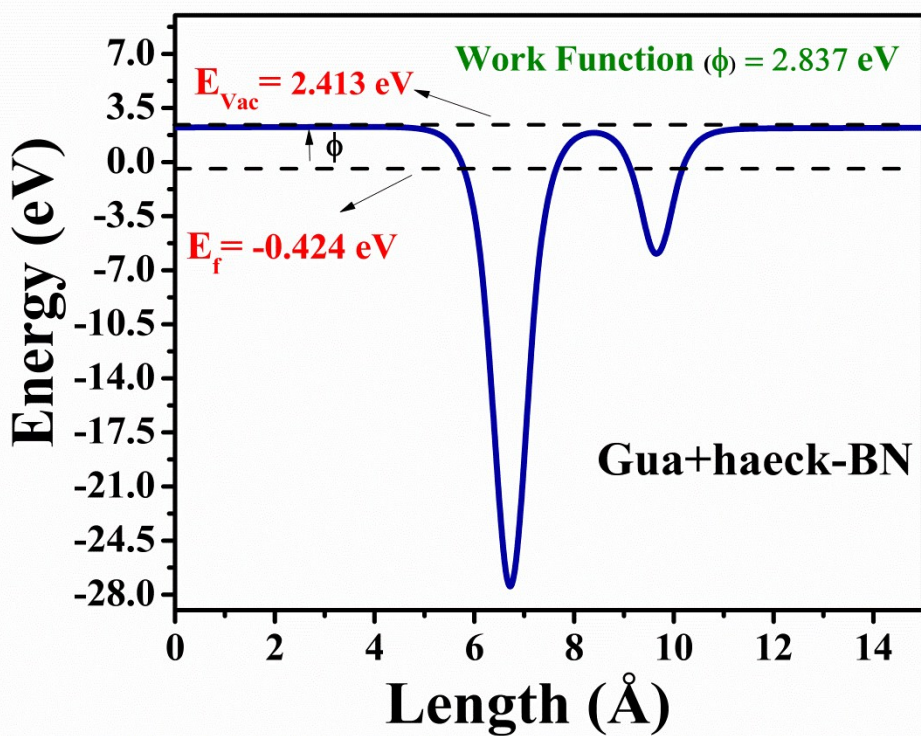


(b)

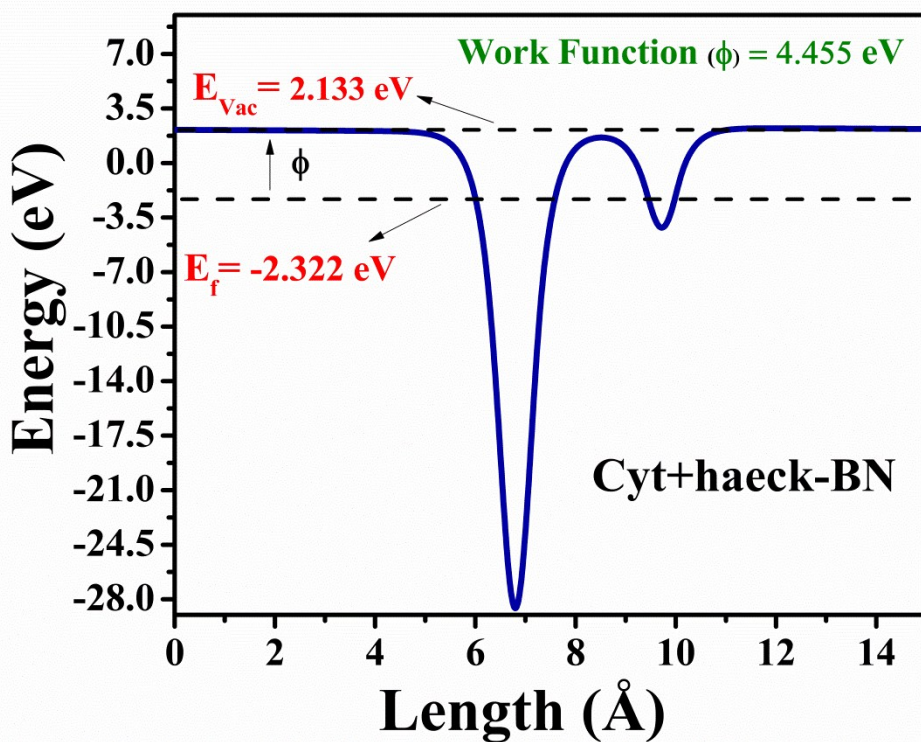




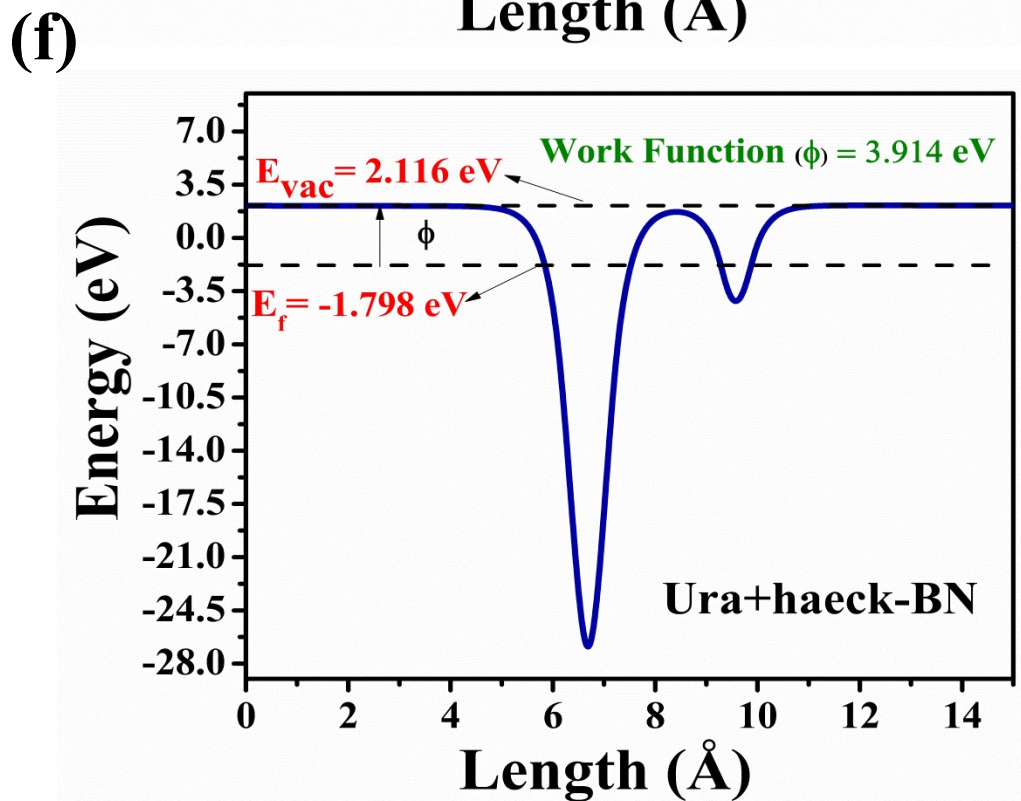
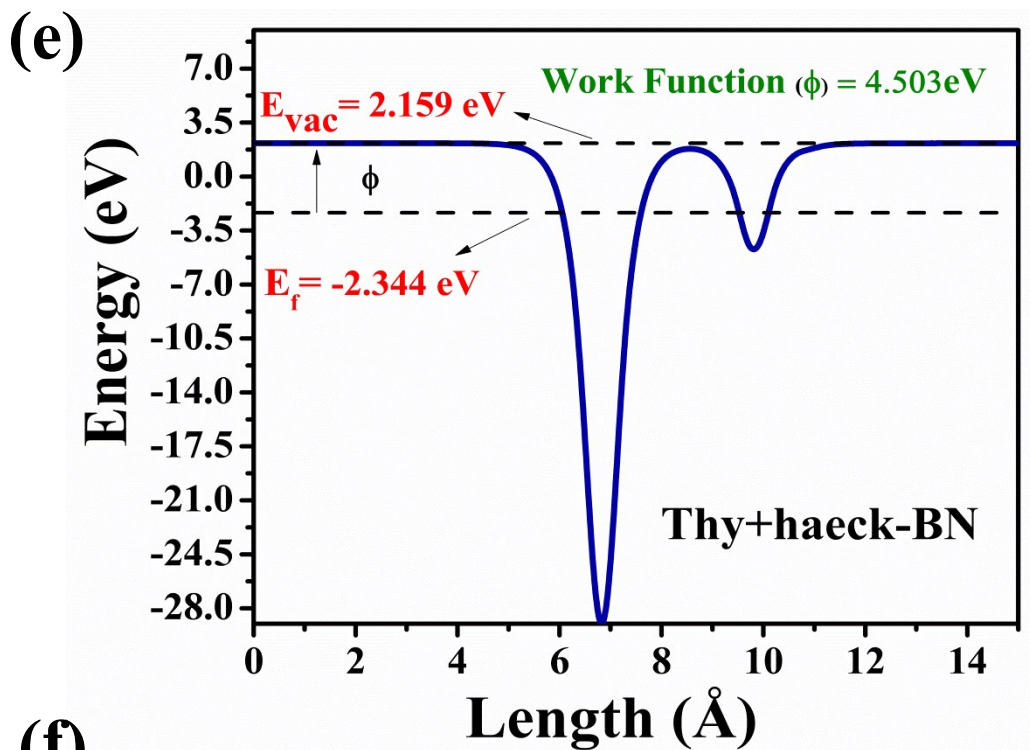
(c)



(d)







**Figure S6:** Work function plot of pristine and nucleobases adsorbed haeck-BN system (a) Pristine, (b) Adenine, (c) Guanine, (d) Cytosine, (e) Thymine and (f) Uracil.