Electronic Supplementary Information (ESI)

Exploring edge functionalised blue phosphorene nanoribbons as novel photocatalysts for water splitting

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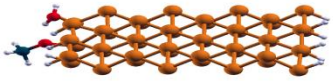
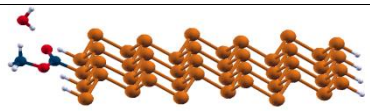
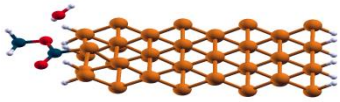
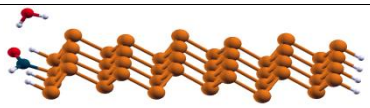
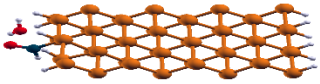
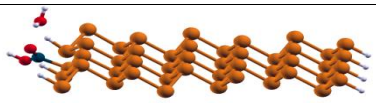
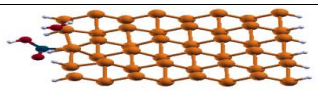
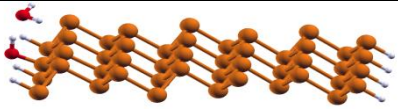
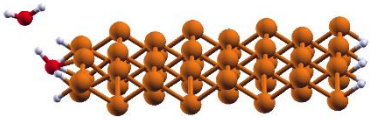
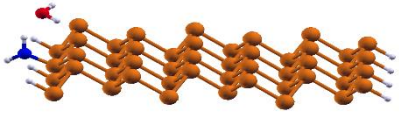
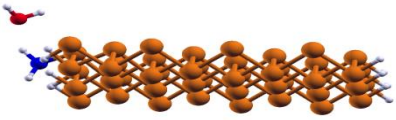
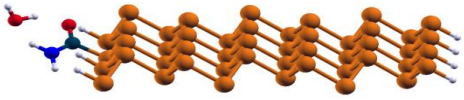
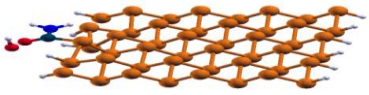
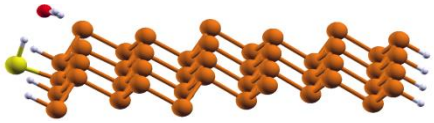
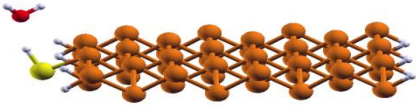
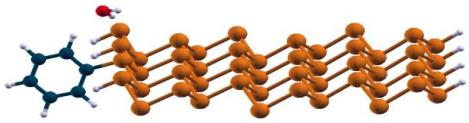
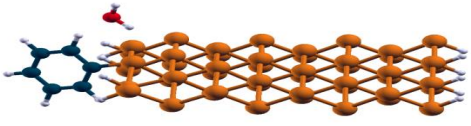
Side view of functionalised zigzag and armchair BPNRs. Tabular form of their adsorption energy, O-H bond length of adsorbed water molecule, symmetric and symmetric stretching frequency. The adsorption energy plot of armchair functionalised BPNRs.

 CH_3O zigzag functionalised BPNR	 CH_3O armchair functionalised BPNR
 $COOCH_3$ zigzag functionalised BPNR	 $COOCH_3$ armchair functionalised BPNR
 CHO zigzag functionalised BPNR	 CHO armchair functionalised BPNR
 COOH zigzag functionalised BPNR	 COOH armchair functionalised BPNR
 OH zigzag functionalised BPNR	 OH armchair functionalised BPNR
 NH_2 zigzag functionalised BPNR	 NH_2 armchair functionalised BPNR
 $CONH_2$ zigzag functionalised BPNR	 $CONH_2$ armchair functionalised BPNR
 SH zigzag functionalised BPNR	 SH armchair functionalised BPNR
	

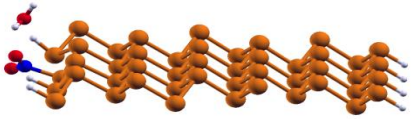
C_6H_5 zigzag functionalised BPNR	C_6H_5 armchair functionalised BPNR
	
NO_2 zigzag functionalised BPNR	NO_2 functionalised BPNR

Fig. S1 Side view of water adsorbed functionalised BPNRs

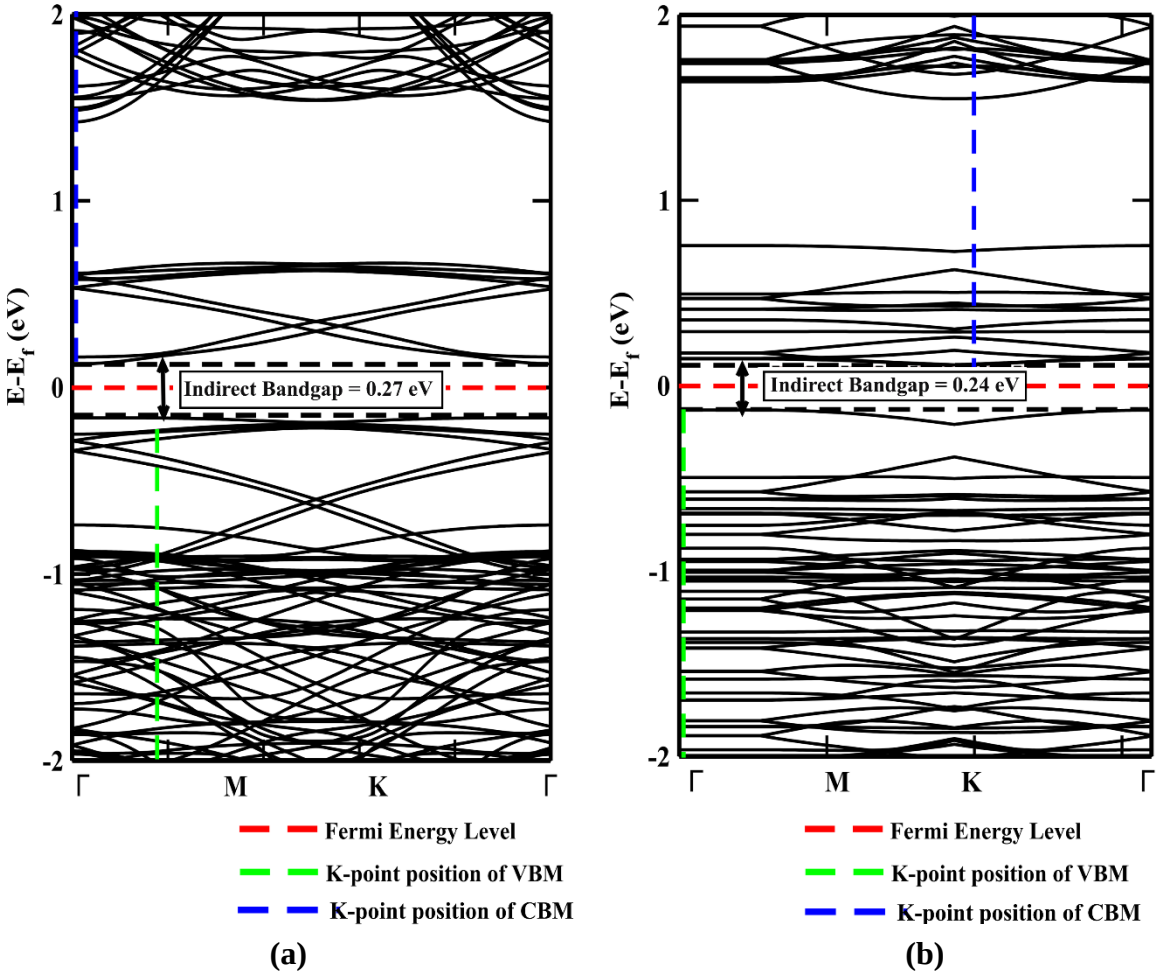
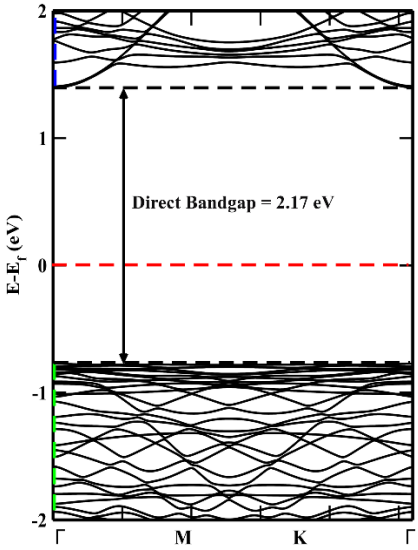
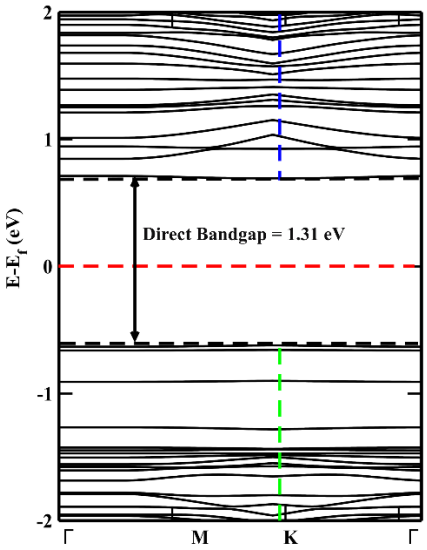


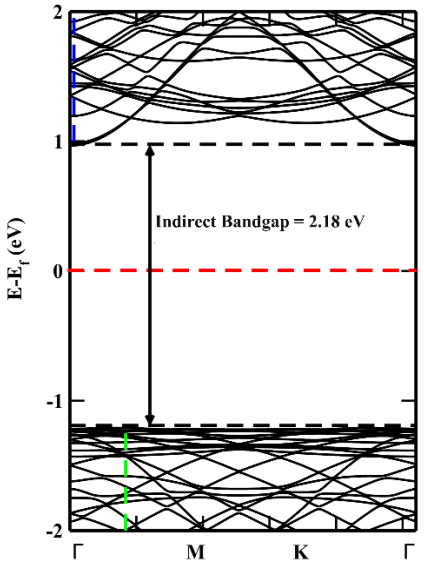
Fig.S2 (a) Band structure of bare zigzag BPNR, (b) Band structure of bare armchair BPNR.



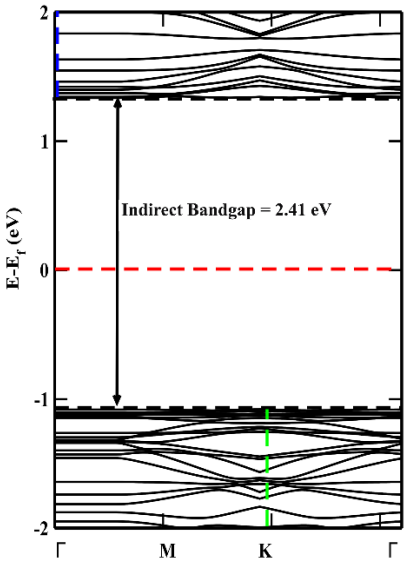
CH_3O functionalised zigzag BPNR



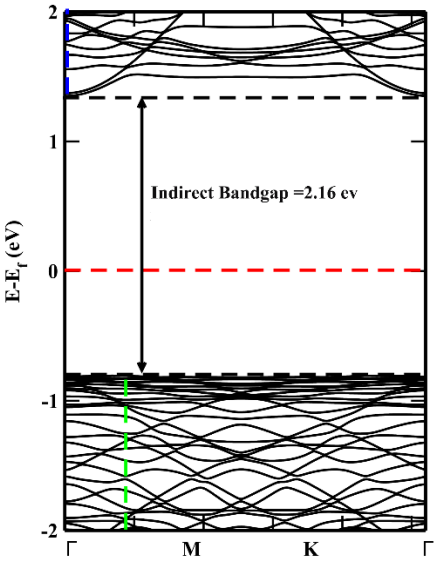
CH_3O functionalised armchair BPNR



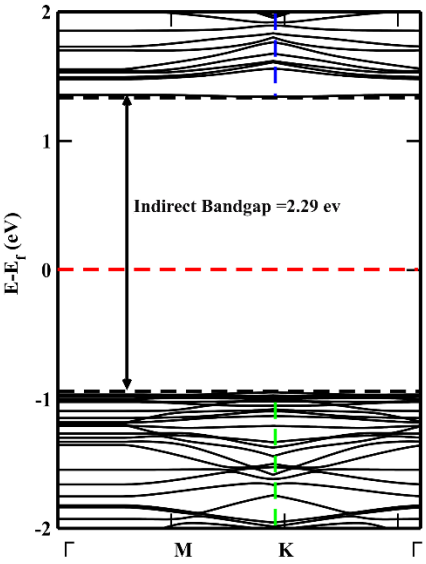
$COOCH_3$ functionalised zigzag BPNR



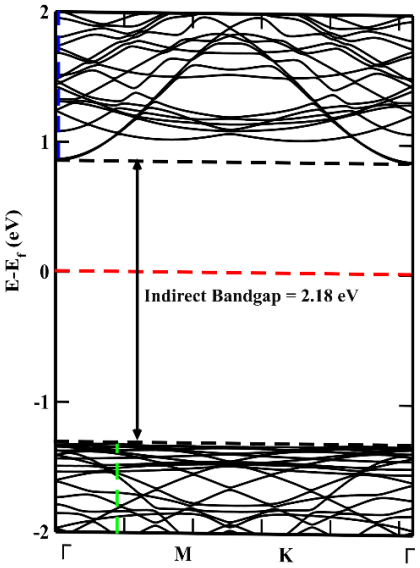
$COOCH_3$ functionalised armchair BPNR



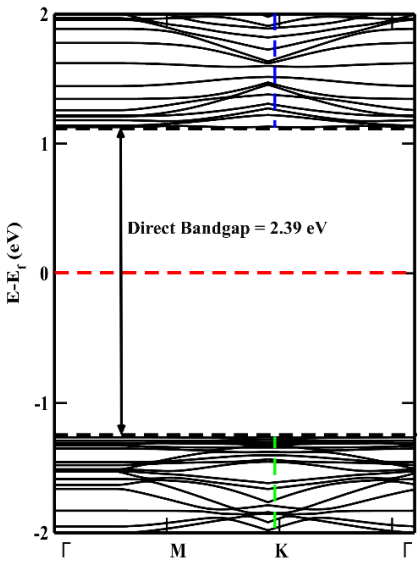
CHO functionalised zigzag BPNR



CHO functionalised armchair BPNR



COOH functionalised zigzag BPNR



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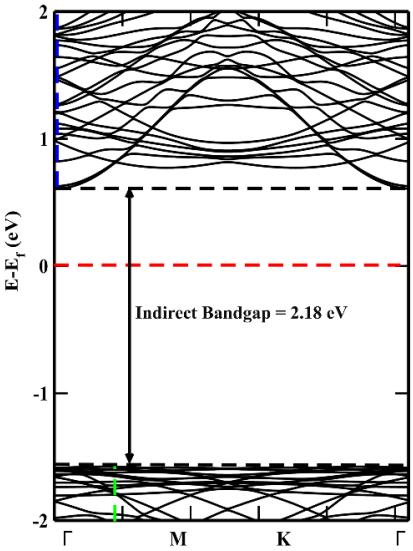

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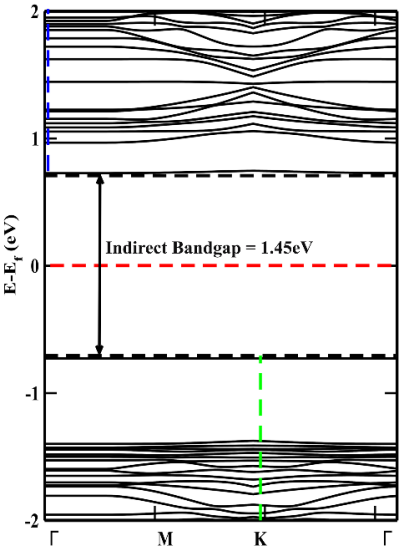
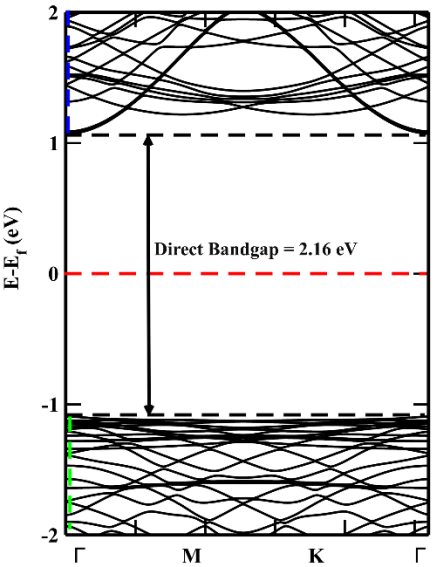
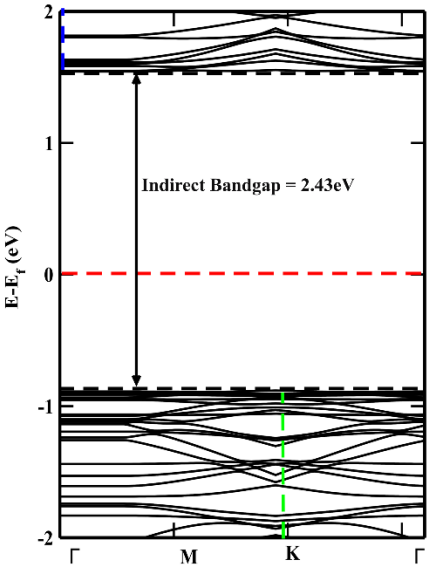


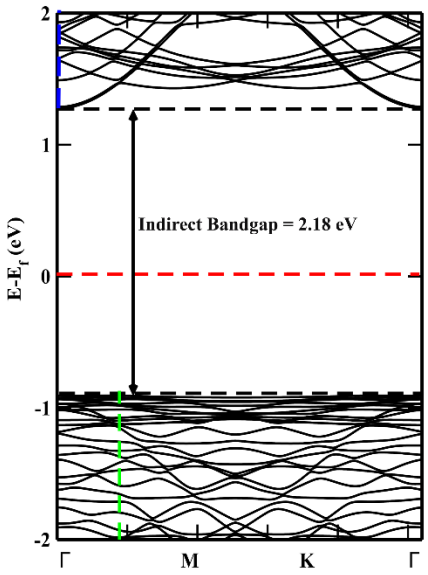
OH functionalised armchair BPNR



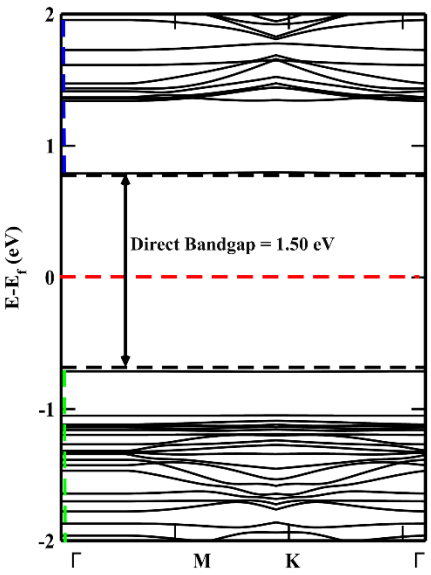
NH_2 functionalised zigzag BPNR



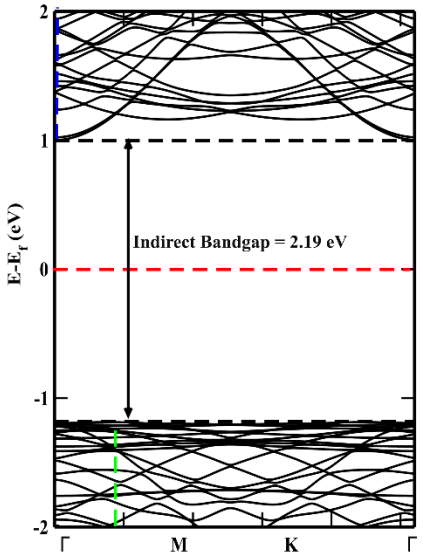
NH_2 functionalised armchair BPNR



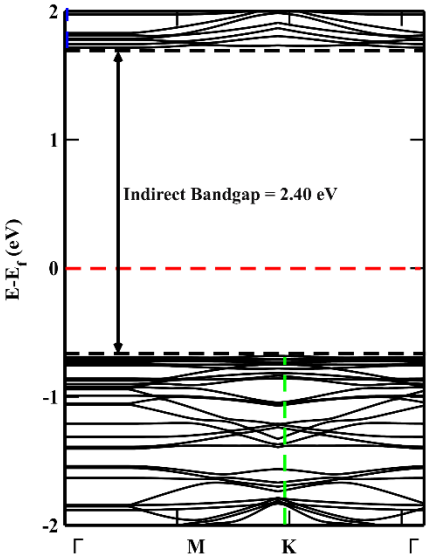
$CONH_2$ functionalised zigzag BPNR



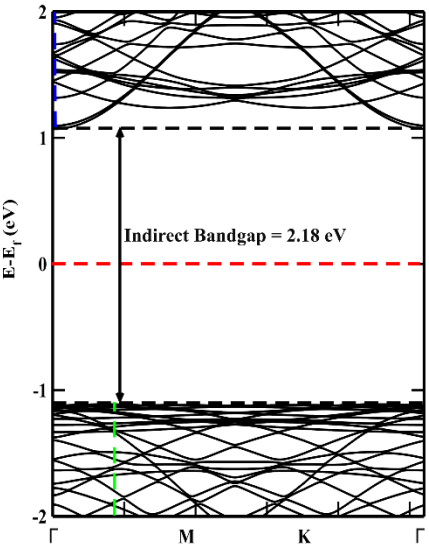
$CONH_2$ functionalised armchair BPNR



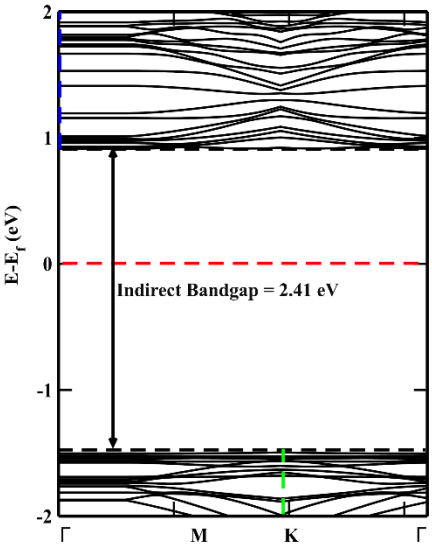
SH functionalised zigzag BPNR



SH functionalised armchair BPNR



C_6H_5 functionalised zigzag BPNR



C_6H_5 functionalised armchair BPNR

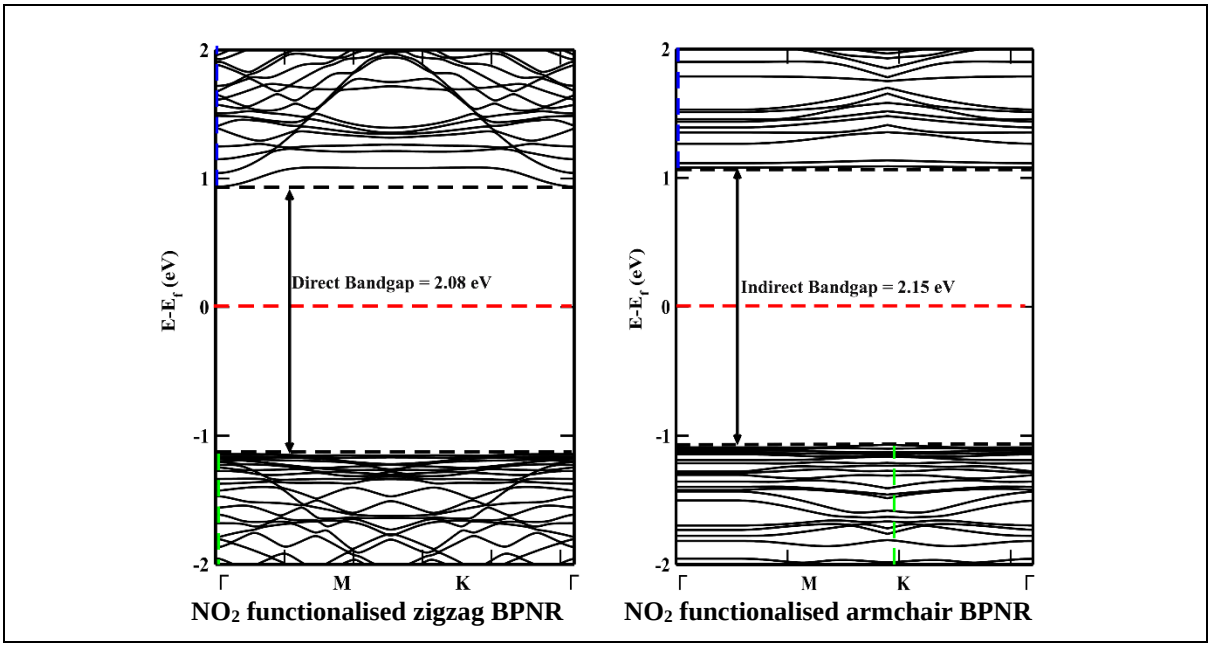


Fig.S3 Band structures of functionalised zigzag and armchair BPNRs.

Table S1: Band edge positions (CBM and VBM) of functionalised BPNRs.

Functional groups	Zigzag functionalised BPNRs		Armchair functionalised BPNRs	
	CBM	VBM	CBM	VBM
CH_3O	-2.644	-4.811	-2.723	-4.036
$COOCH_3$	-2.633	-4.809	-2.376	-4.788
CHO	-2.729	-4.887	-2.596	-4.887
COOH	-2.650	-4.829	-2.383	-4.774
OH	-2.673	-4.856	-2.612	-4.066
NH_2	-2.589	-4.753	-2.327	-4.751
$CONH_2$	-2.594	-4.776	-2.930	-4.433
SH	-2.658	-4.847	-2.404	-4.802
C_6H_5	-2.611	-4.792	-2.327	-4.736
NO_2	-2.864	-4.944	-2.730	-4.879

Table S2: Adsorption energy, O-H bond length of zigzag functionalised water adsorbed BPNRs

FUNCTIONAL GROUP	SITES	ADSORPTION ENERGY (eV)	O-H-I BOND LENGTH(Å)	O-H-II BOND LENGTH (Å)
CH_3O	A	-0.842	0.989	0.966
	B	-0.568	0.982	0.981
	C	-0.479	0.978	0.974
	D	-0.456	0.976	0.970
$COOCH_3$	A	-0.677	0.984	0.968
	B	-0.582	0.983	0.979
	C	-0.568	0.980	0.979
	D	-0.586	0.984	0.980
CHO	A	-0.514	0.973	0.971
	B	-0.433	0.977	0.969
	C	-0.576	0.981	0.980
	D	-0.590	0.981	0.980
COOH	A	-0.637	0.979	0.968
	B	-0.513	0.977	0.977
	C	-0.565	0.982	0.981
	D	-0.579	0.981	0.980
OH	A	-0.959	0.989	0.974
	B	-0.578	0.983	0.980
	C	-0.568	0.982	0.980
	D	-0.458	0.976	0.971
NH_2	A	-0.794	0.986	0.983
	B	-0.587	0.982	0.980
	C	-0.573	0.981	0.981
	D	-0.584	0.980	0.980
$CONH_2$	A	-0.979	0.999	0.965
	B	-0.550	0.983	0.981
	C	-0.435	0.977	0.971
	D	-0.565	0.983	0.979
SH	A	-0.787	0.989	0.975
	B	-0.567	0.982	0.980
	C	-0.450	0.977	0.970
	D	-0.582	0.983	0.980
C_6H_5	A	-0.665	0.984	0.972
	B	-0.553	0.983	0.979
	C	-0.440	0.978	0.971
	D	-0.574	0.982	0.981
NO_2	A	-0.738	0.980	0.968
	B	-0.452	0.978	0.971
	C	-0.590	0.982	0.980
	D	-0.601	0.983	0.980

Table S3: Adsorption energy, O-H bond length of armchair functionalised water adsorbed BPNRs

FUNCTIONAL GROUP	SITES	ADSORPTION ENERGY (eV)	O-H-I BOND LENGTH(Å)	O-H-II BOND LENGTH (Å)
CH_3O	A	-0.766	0.987	0.969
	B	-0.565	0.985	0.971
	C	-0.5	0.982	0.969
	D	-0.542	0.982	0.980
$COOCH_3$	A	-0.424	0.974	0.968
	B	-0.526	0.981	0.978
	C	-0.469	0.977	0.975
	D	-0.479	0.977	0.976
CHO	A	-0.876	0.991	0.967
	B	-0.636	0.977	0.977
	C	-0.476	0.976	0.976
	D	-0.558	0.983	0.979
COOH	A	-0.652	0.977	0.974
	B	-0.439	0.976	0.973
	C	-0.483	0.976	0.976
	D	-0.483	0.977	0.976
OH	A	-0.690	0.990	0.969
	B	-0.472	0.976	0.969
	C	-0.577	0.983	0.981
	D	-0.481	0.976	0.975
NH_2	A	-0.545	0.977	0.968
	B	-0.572	0.981	0.981
	C	-0.560	0.981	0.980
	D	-0.490	0.977	0.975
$CONH_2$	A	-0.705	0.991	0.968
	B	-0.442	0.976	0.974
	C	-0.549	0.981	0.980
	D	-0.549	0.984	0.972
SH	A	-0.516	0.980	0.968
	B	-0.497	0.976	0.975
	C	-0.492	0.977	0.974
	D	-0.488	0.978	0.974
C_6H_5	A	-0.506	0.979	0.975
	B	-0.473	0.976	0.975
	C	-0.482	0.976	0.976
	D	-0.466	0.976	0.975
NO_2	A	-0.466	0.972	0.975
	B	-0.417	0.977	0.972
	C	-0.479	0.976	0.974
	D	-0.484	0.977	0.974