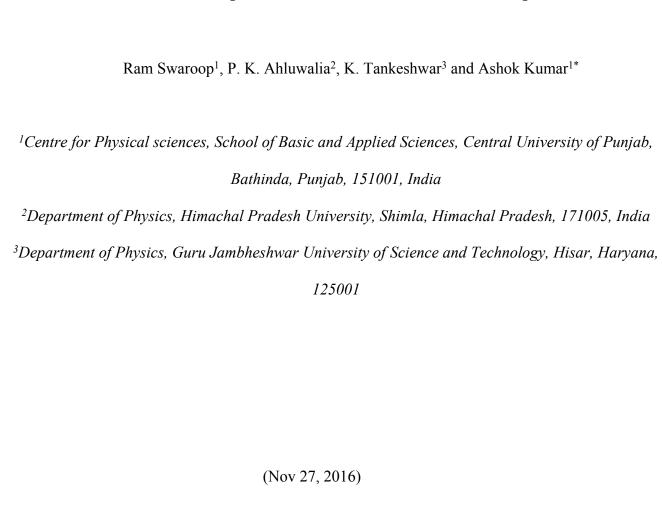
Supplementary Information

Ultra-narrow Blue Phosphorene Nanoribbons for Tunable Optoelectronics



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H-ABPNR H-ZBPNR

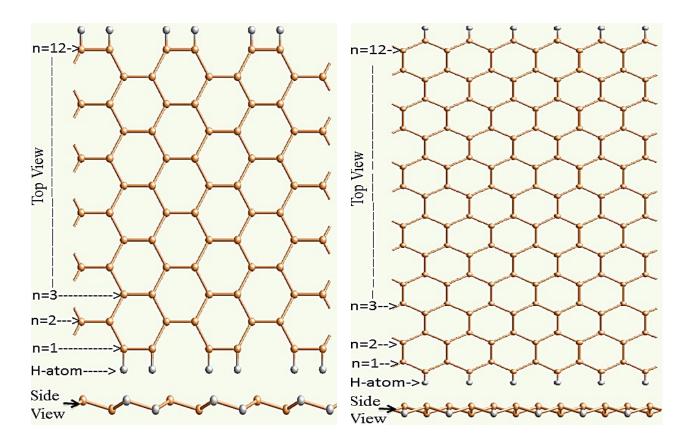


Figure S1: Top and Side view of H-ABPNR and H- ZBPNR for the widest ribbon (n=12) considered in the study.

Initial structures

Relaxed structures

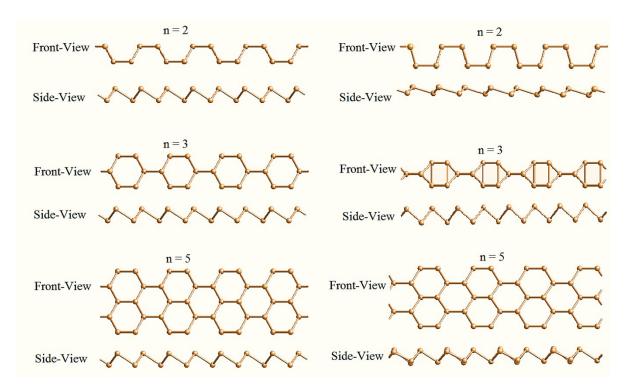


Figure S2: Inital and fully relaxed structures of ABPNR at width n = 2, 3, 5. The reconstruction of edge atoms can be seen in relaxed structures.

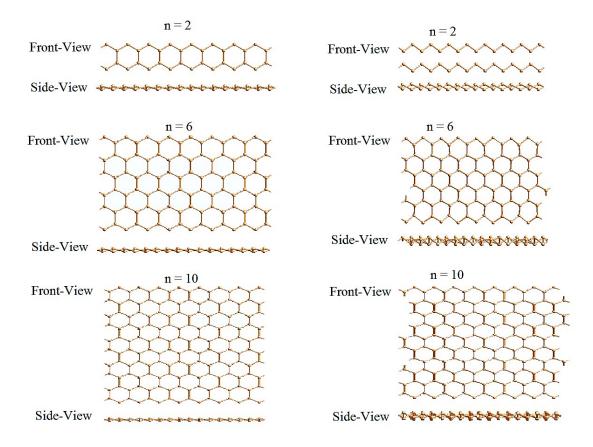


Figure S3: Inital and fully relaxed structures of ZBPNR at width n = 2, 3, 5. The reconstruction of edge atoms can be seen in relaxed structures.

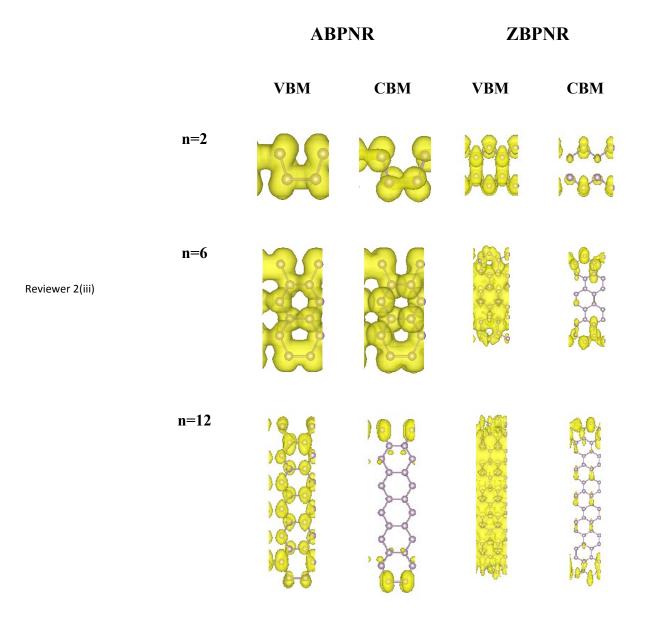


Figure S4: Valance band maxumum (VBM) and conduction band minimum (CBM) charge density for width n=2, 6 and 12 of bare BPNRs. The iosurface value is set at 10⁻³ e/Å³.

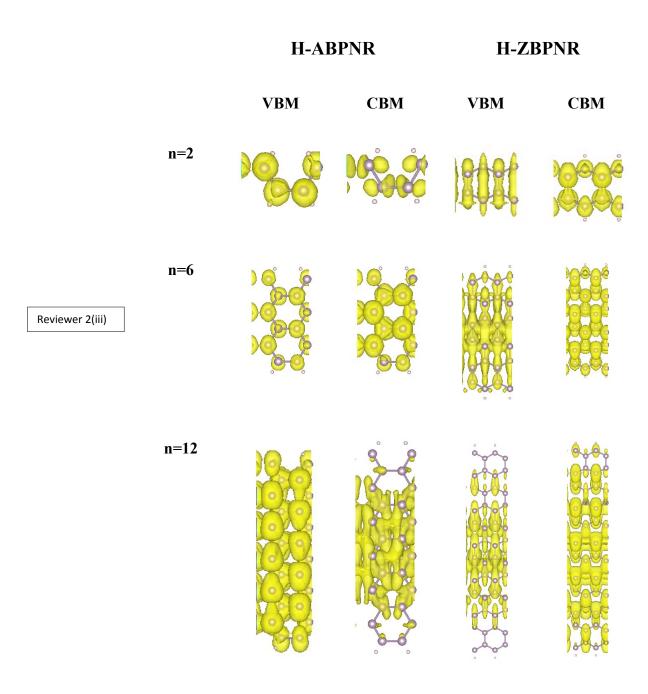


Figure S5: Valance band maxumum (VBM) and conduction band minimum (CBM) charge density for width n=2, 6 and 12 of passivated BPNRs. The iosurface value is set at 10^{-7} e/Å³.

Table T1: Plasmonic energy (eV) of $\pi+\sigma$ structure peak for smallest width (n=2) and widest width (n=12) BPNRs. The plasmonic energy at 2% and at ultimate tensile strength (UTS) of widest width BPNR is also given.

	π+σ plasmonic energy (eV)			
	n=2	n=12	2%	at UTS
ABPNR	5.8	8.4	8.3	6.3
H-ABPNR	6.8	8.8	8.6	6.5
ZBPNR	6.0	8.6	8.4	6.4
H-ZBPNR	6.3	8.5	8.2	6.3