Electronic Supplementary Information (ESI)

Band offsets in new BN/BX (X = P, As, Sb) lateral heterostructures based on bond-orbital theory

Wenhan Zhou,[†a] Xuhai Liu,[†a] Xuemin Hu,[a] Shengli Zhang,[*a] Chunyi Zhi,[b] Bo Cai,[a] Shiying Guo,[a] Xiufeng Song,[a] Zhi Li,[a] Haibo Zeng[*a]

[a]MIIT Key Laboratory of Advanced Display Materials and Devices, Ministry of Industry and Information Technology, Institute of Optoelectronics & Nanomaterials, Nanjing University of Science and Technology, Nanjing, 210094, China.

[b]Department of Materials Science and Engineering, City University of Hong Kong, 83 Tat Chee Avenue, Kowloon, Hong Kong 999077, China.

[†]These authors contributed equally.

[*]Corresponding authors and E-mail: zhangslvip@njust.edu.cn zeng.haibo@njust.edu.cn

TABLE SI. Bond length, lattice constant, VBM, and CBM values of BN and BX (X = P, As, Sb) monolayers.

Material	Bond Lengths (Å)	Lattice Constants (Å)	VBM (eV)		CBM (eV)	
			PBE	HSE	PBE	HSE
BN	1.45	2.51	-5.80	-6.56	-1.14	-0.88
BP	1.85	3.21	-5.08	-5.43	-4.18	-3.84
BAs	1.96	3.39	-4.89	-5.21	-4.13	-3.78
BSb	2.15	3.73	-4.49	-4.83	-4.17	-3.92

TABLE SII. Bond length and lattice constant of $(BN)_n(BX)_n$ (X = P, As, Sb; n = 2, 4, 6, 8) lateral heterojunctions.

LHS (Zigzag)	Bond Lengths (Å)		Lattice Constants (Å)	LHS (Armchair)	Bond Lengths (Å)		Lattice Constants (Å)
	B-N	B-X			B-N	B-X	
$(BN)_2(BP)_2$	1.527	1.800	2.830	$(BN)_2(BP)_2$	1.482	1.849	2.832
$(BN)_4(BP)_4$	1.529	1.793	2.841	$(BN)_4(BP)_4$	1.506	1.822	2.823
$(BN)_6(BP)_6$	1.530	1.791	2.841	$(BN)_6(BP)_6$	1.514	1.811	2.822
$(BN)_8(BP)_8$	1.531	1.789	2.842	$(BN)_8(BP)_8$	1.518	1.807	2.822
$(BN)_2(BAs)_2$	1.549	1.891	2.923	$(BN)_2(BAs)_2$	1.488	1.950	2.904
$(BN)_2(BSb)_2$	1.574	2.087	3.020	$(BN)_2(BSb)_2$	1.503	2.162	3.032

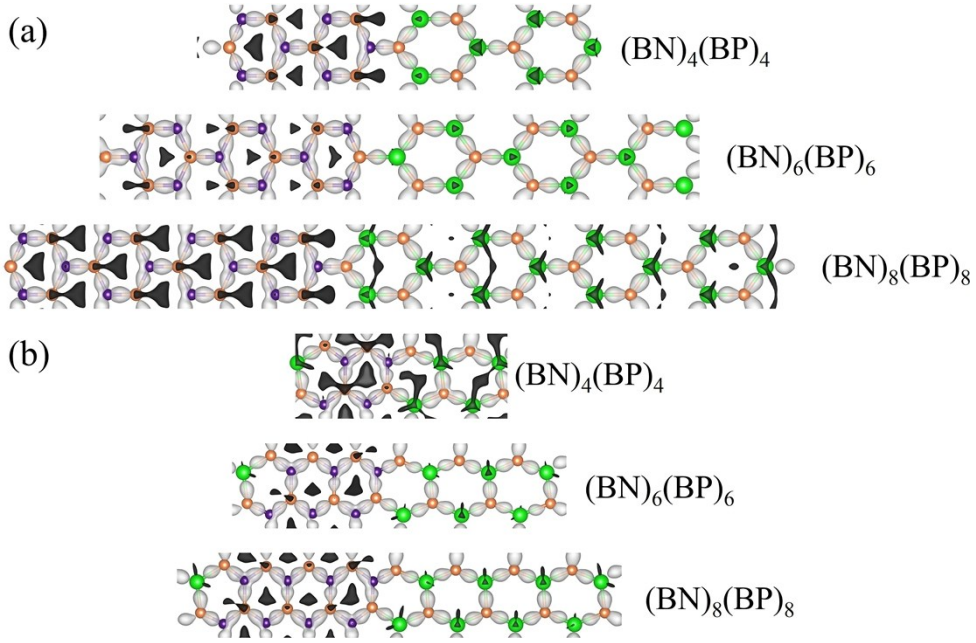

Fig. S1 Deformation charge density of $(BN)_n(BX)_n$ LHS (n =4, 6, 8) along zigzag (a) and armchair (b) directions, respectively. White and black color refer to electron accumulation and depletion region, respectively.

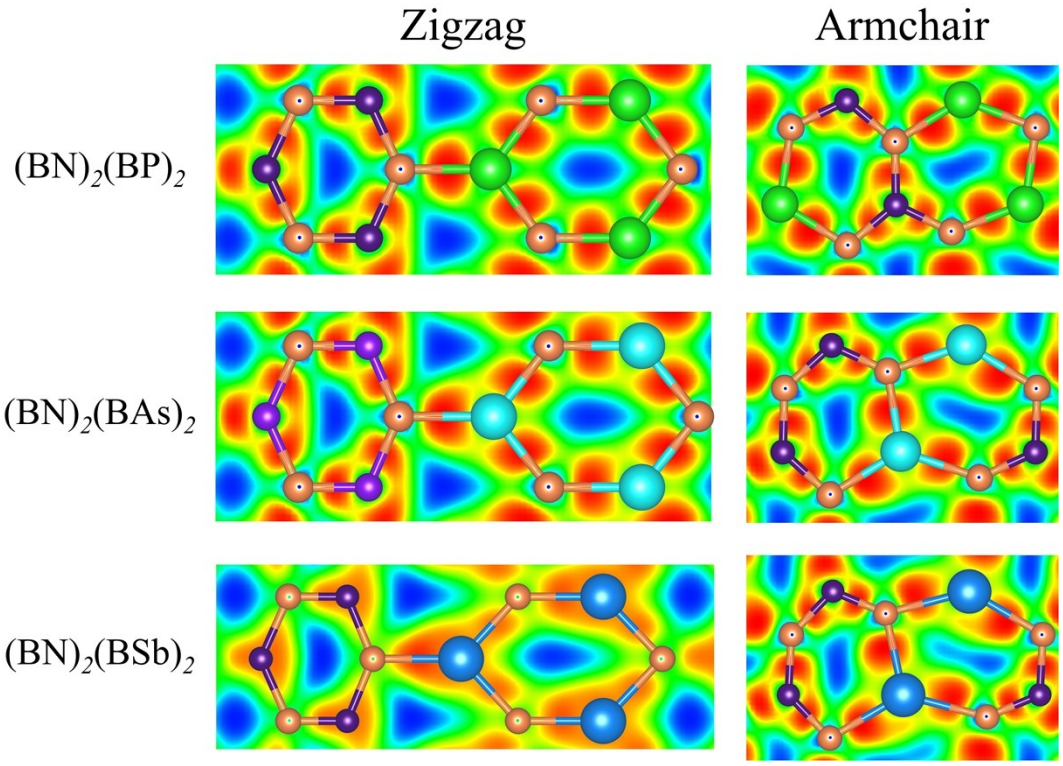

Fig. S2 Electron localization functions (ELFs) of the B-N and B-X bonds in $(BN)_2(BX)_2$ LHS.

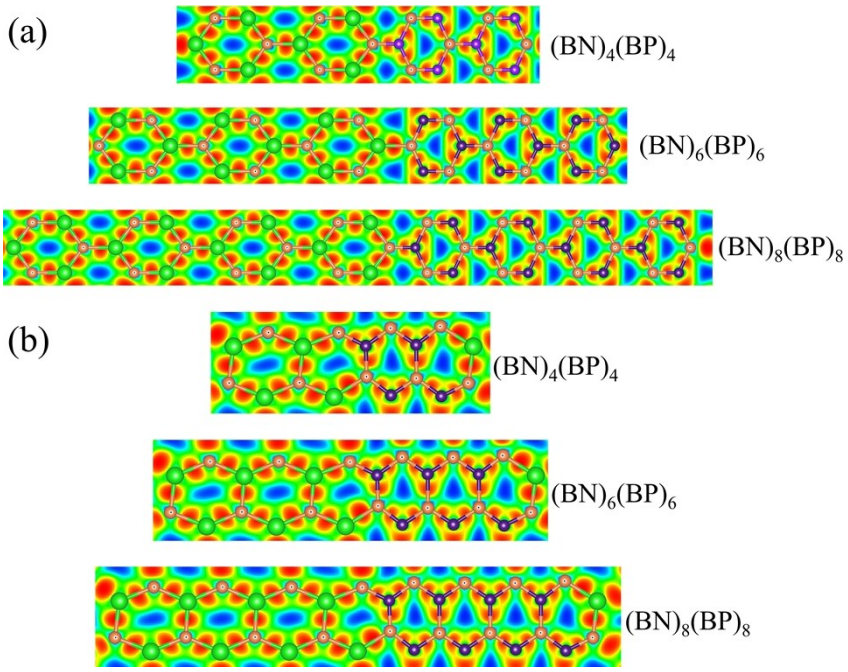

Fig. S3 Electron localization functions (ELFs) of the B-N and B-P bonds in $(BN)_n(BP)_n$ LHS (n =4, 6, 8).

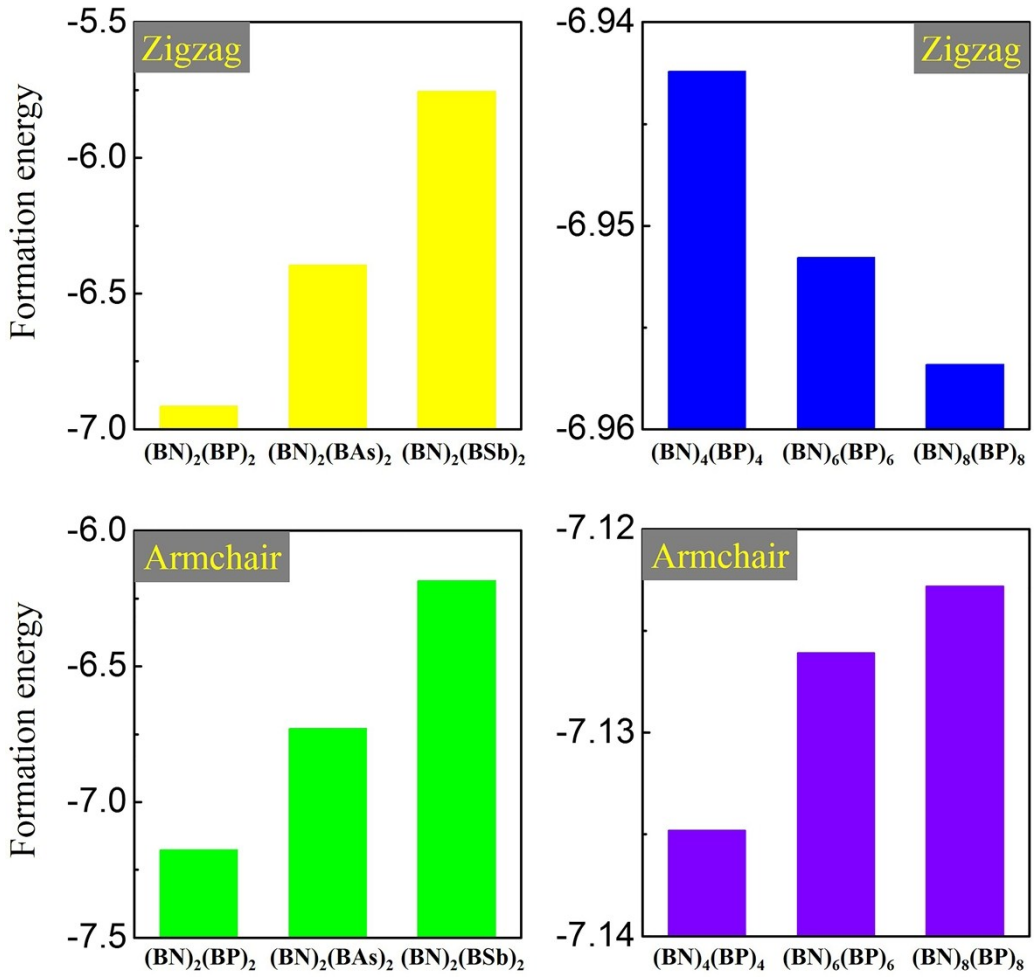

Fig. S4 Formation energy of $(BN)_n(BX)_n$ LHS (X = P, As, Sb; n = 2, 4, 6, 8).

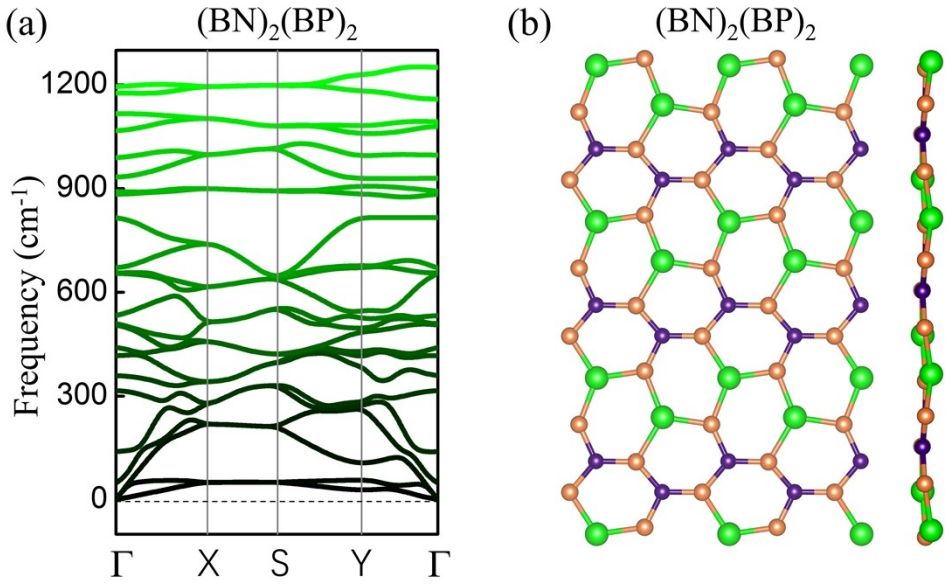

Fig. S5 (a) Calculated phonon dispersion spectra of the armchair $(BN)_2(BP)_2$ LHS. (b) Top (left panel) and side (right panel) views of the snapshots from the molecules dynamic simulation of atomic structures for the armchair $(BN)_2(BP)_2$ LHS at the temperature of 300 K.

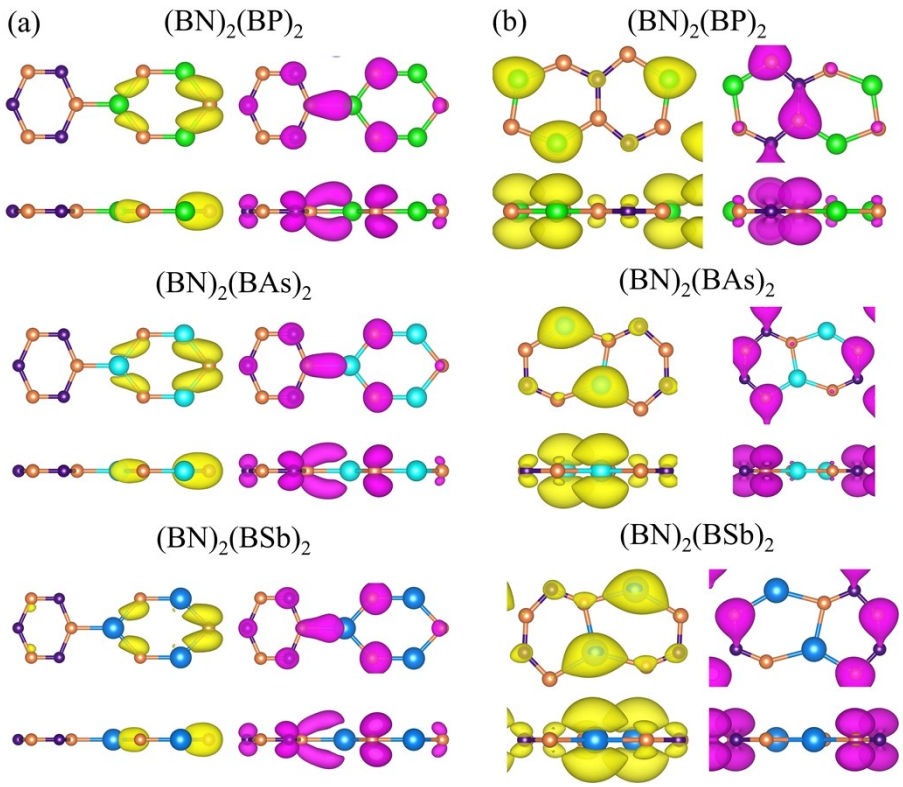

Fig. S6 Iso-surfaces of partial charge densities for the VBM and CBM of zigzag (a) and armchair (b) $(BN)_2(BX)_2$ LHS.

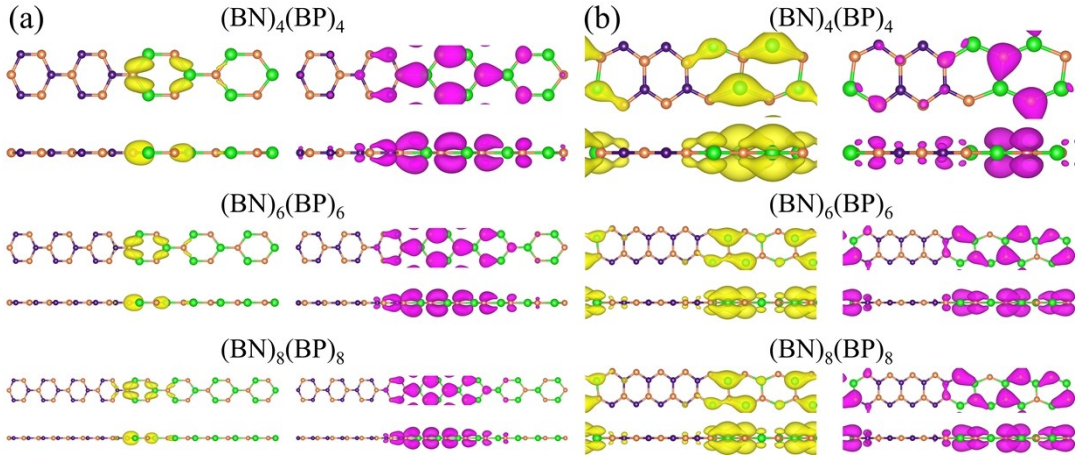

Fig. S7 Iso-surfaces of partial charge densities for the VBM and CBM of zigzag (a) and armchair (b) $(BN)_n(BP)_n$ LHS (n =4, 6, 8).