Supporting Information

The Bulk Photovoltaic Effect in the One-Dimensional Interface of Graphene/BN Superlattice

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Table 1. The lattice parameter b (Å), C-B, and C-N bond length (Å) at the interface of armchair graphene/BN SLs with different widths N. The B–N and C-C bond length change relative to that of the pristine graphene and BN (%).

Chain (N)	Lattice parameter b (Å)	C-B (Å)	C-N (Å)	Δ(B–N)/B–N_{pri} (%)	Δ(C–C)/C–C_{pri} (%)
1	4.321	1.517	1.393	−0.069	0.070
2	4.312	1.517	1.403	−0.207	0.491
3	4.312	1.518	1.406	−0.551	0.140
4	4.312	1.516	1.406	−0.620	0.140
5	4.310	1.517	1.406	−0.690	0.351
6	4.310	1.517	1.407	−0.690	0.280
7	4.319	1.507	1.399	−0.552	0.561
8	4.318	1.506	1.398	−1.103	0.632
9	4.319	1.507	1.399	−1.103	0.561

Table S2. The bandgap, bandgap type, and the first peak value of σ^{yyy} of graphene/BN SLs with different widths.

	Chain (N)	Band gap (eV)	Bandgap type	σ^{yyy} (μA/V²)
$C_4B_2N_2$	1	1.136	Direct	21.410
	2	1.230	Indirect	32.315
	3	1.327	Direct	15.627
	4	0.579	Direct	157.543

	5	0.658	Direct	117.797
	6	0.862	Direct	30.568
	7	0.455	Direct	184.131
	8	0.476	Direct	143.431
	9	0.651	Direct	85.853
$C_2B_3N_3$	1	1.991	Indirect	26.397
$C_6B_1N_1$	1	1.046	Direct	21.672

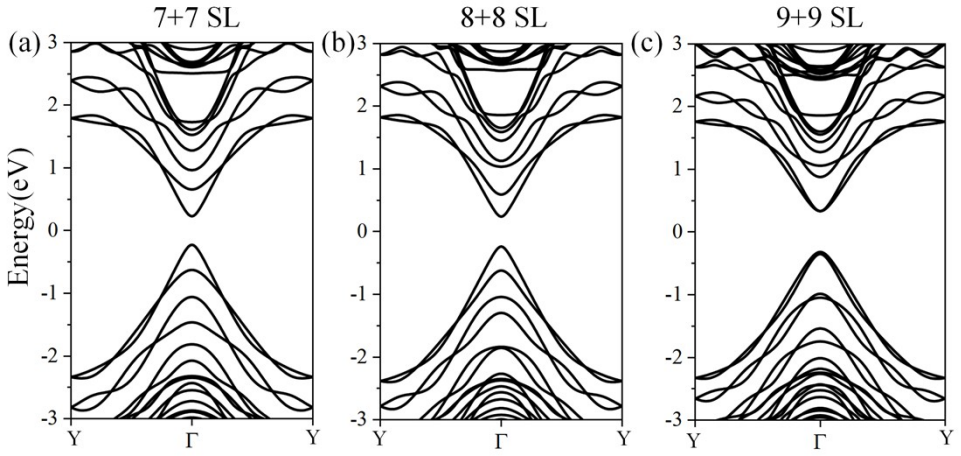

Figure S1 The electric band structure of the 7+7, 8+8, 9+9 SL. As the width N of the nanoribbon increases, the graphene/BN armchair SL can be regarded as one-dimensional materials, and the high-symmetry *k*-path transforms into Y–Γ–Y.

Figure S2 shows the orbital-resolved band structure of 1+1, 2+2, and 3+3 armchair SLs. For 3+3 armchair SL, the weight of C-, B-, and N-p_z orbitals at the Γ point is significantly larger than that of other high-symmetry points, indicating a higher density of states at the Γ point. The relatively flat bands are seen at the Γ point due to electronic state condensation. In contrast, for 1+1 and 2+2 armchair SLs, the p_z is dominant near the K point. Furthermore, compared to the band structure of 1+1 and 2+2 armchair SLs, strong interactions between VBM and VB–2, as well as CBM and CB–2, are evident in the 3+3 case, further confirming the effect of BZ folding.

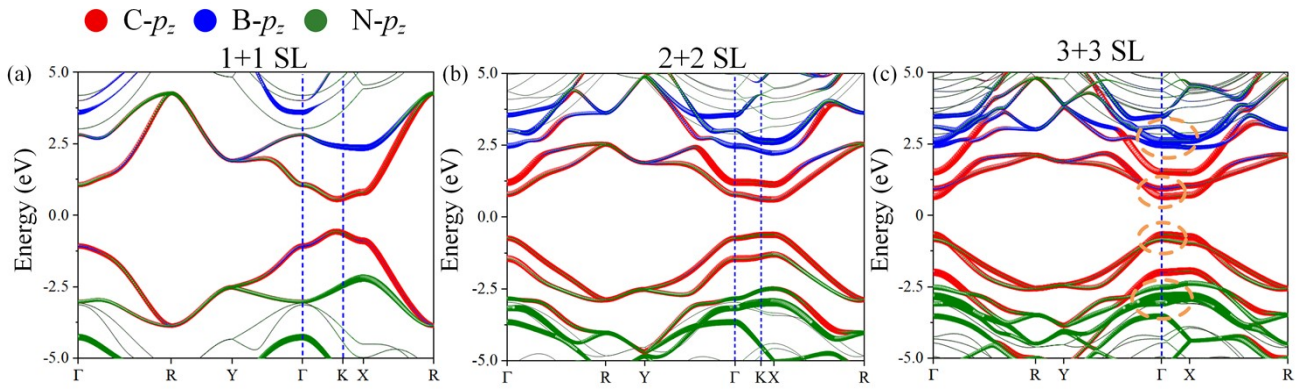

Figure S2 The orbital-resolved band structure of (a) 1+1, (b) 2+2, (c) 3+3 armchair SLs. Red, blue, and green spheres denote the C-, B-, and N-p_z orbital contribution, with the sphere size corresponding to its weight. The orange circles highlight regions with high p_z orbital weight in the 3+3 SL.

The charge transfer at the 1D interface can be characterized by the charge density difference, as shown in Figure S3, where yellow and blue regions indicate electron gain and loss, respectively. Significant charge redistribution is observed across the interface in Figure S3, consistent with the electronegativity differences among C (2.55), B (2.04), and N (3.04) atoms. Specifically, for the C-N bonds at the interface, the higher electronegativity of N compared to C results in electron accumulation around N (yellow regions) and depletion around C (blue regions). Conversely, for the C-B bonds at the interface, the higher electronegativity of C relative to B causes electron accumulation near C and depletion near B. This charge transfer provides clear evidence of stable chemical bonding formation at the interface.

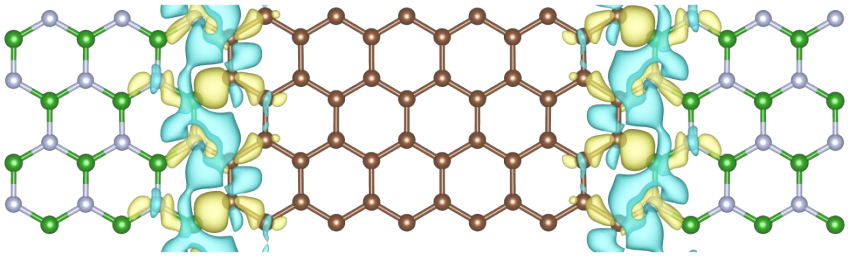

Figure S3. The charge density difference of 6+6 graphene/BN armchair SL.

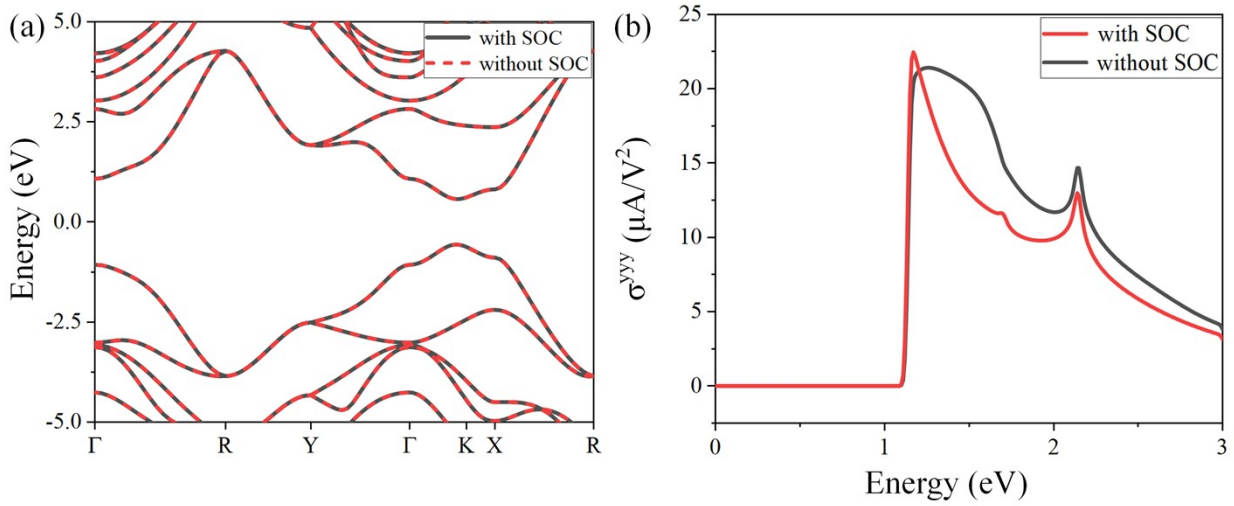

Figure S4 (a) The calculated energy band structure, and (b) the shift current of the 1+1 graphene/BN armchair SL with spin-orbit coupling (SOC) and without SOC.

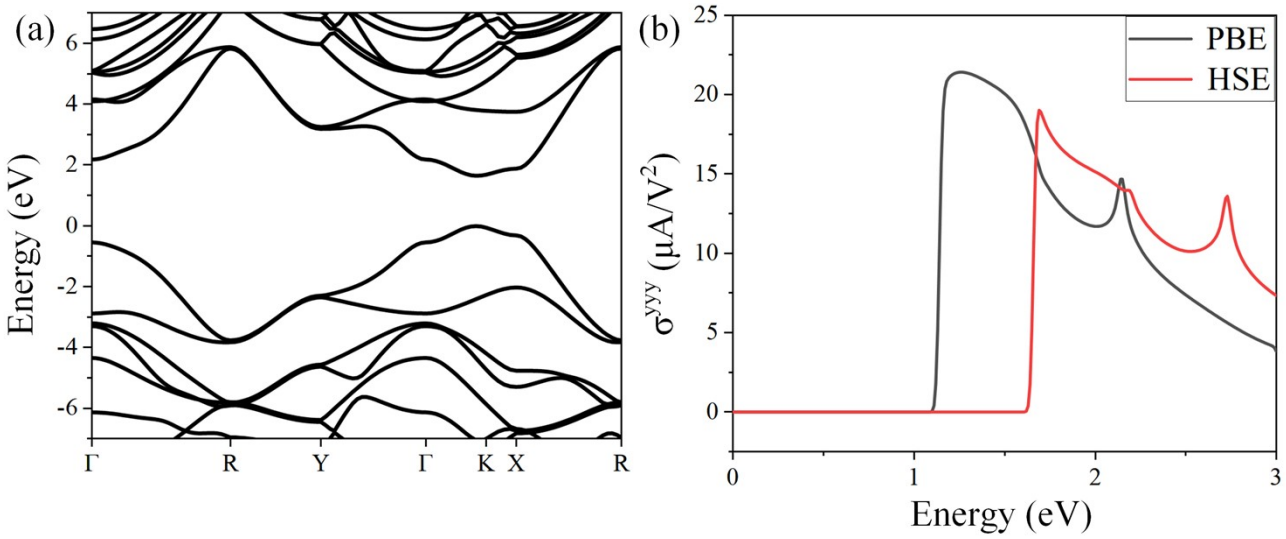

Figure S5 (a) The calculated energy band structure, and (b) the shift current of the 1+1 graphene/BN armchair SL, obtained using the HSE06 functional.

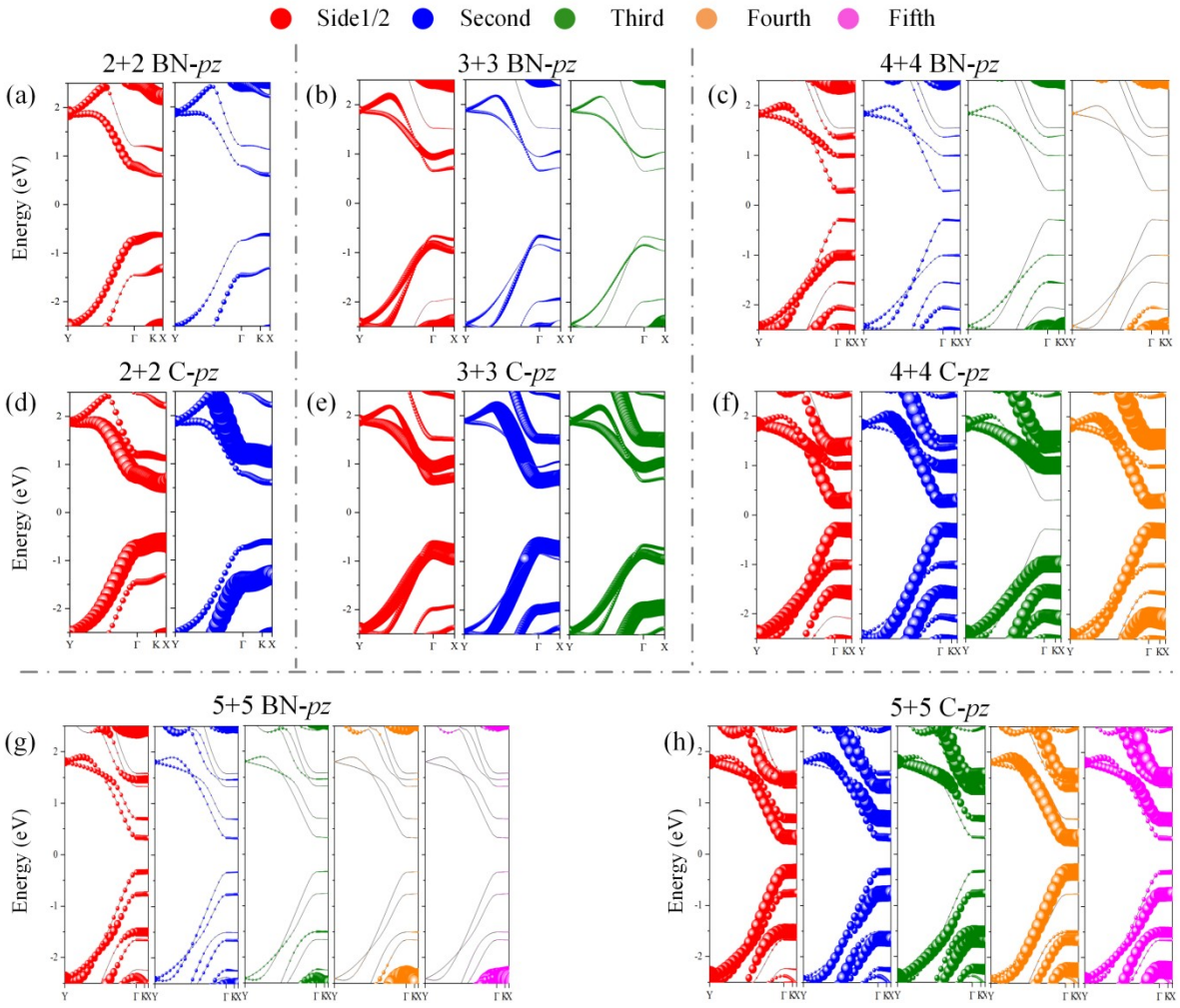

Figure S6 (a-h) The p_z orbital-resolved band structure of the graphene/BN armchair SLs with varying width (N=2-5), with red, blue, green, orange, and magenta dotted lines representing the BN-p_z, and C-p_z orbitals of the 1-5 atomic row, respectively.

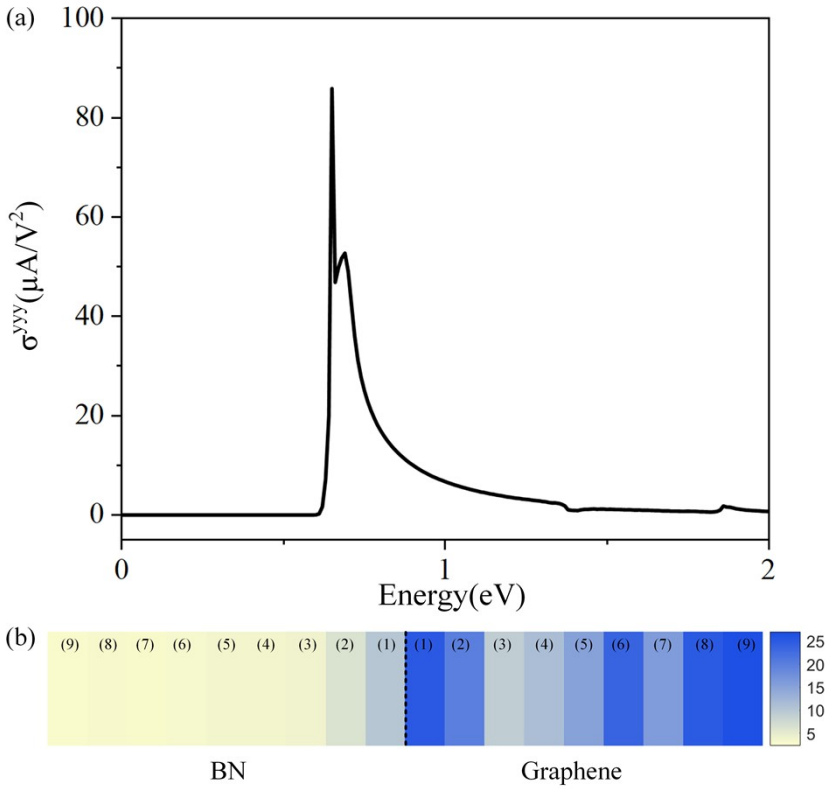

Figure S7 (a) The shift current conductance σ^{yyy} and (b) the heat map of σ^{yyy} contributed by each atomic rows in the 9+9 graphene/BN armchair SLs at the incident photon energy of 0.70 eV.

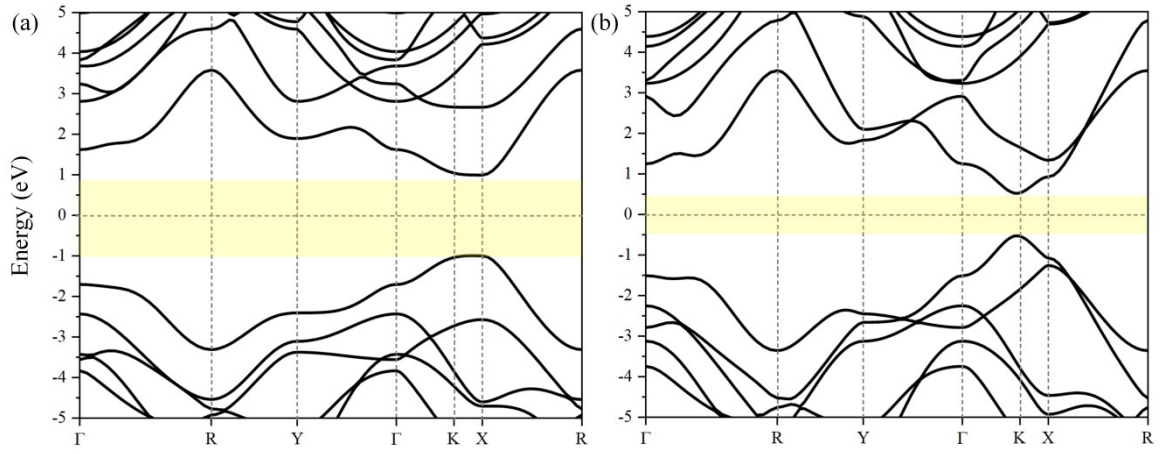

Figure S8 The calculated energy band of the 1+1 armchair (a) $C_2B_3N_3$, (b) $C_6B_1N_1$ SLs.