Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Observation of Dirac state in borophene hetero-bilayer by Cr intercalation

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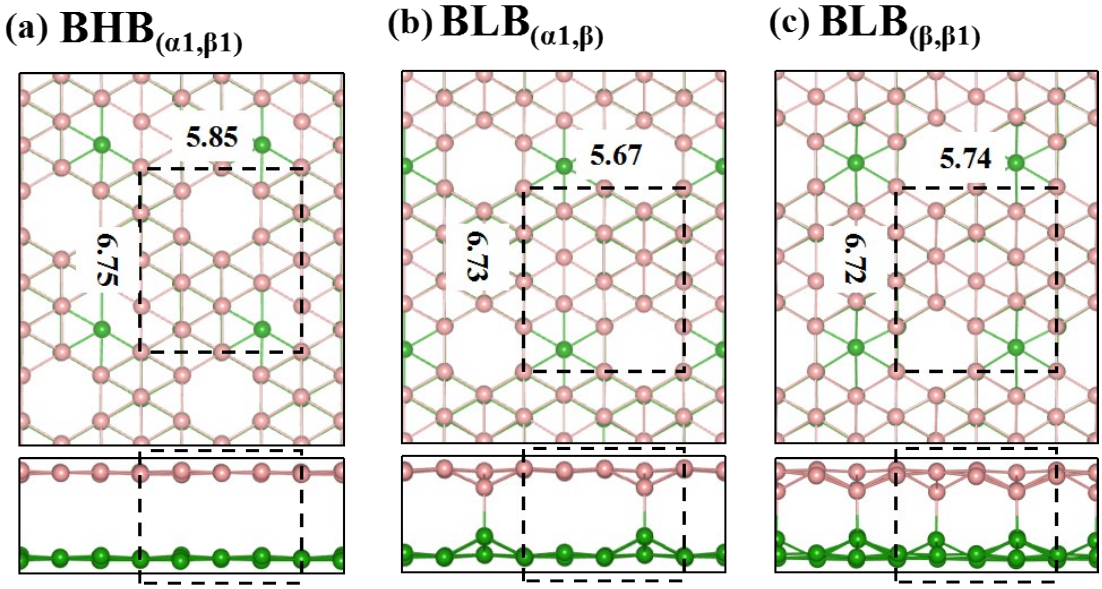

Fig. S1 Top and side view of optimized structures of bilayer (α_1,β_1)-, (α_1,β)- and (β,β_1)- boron sheets.

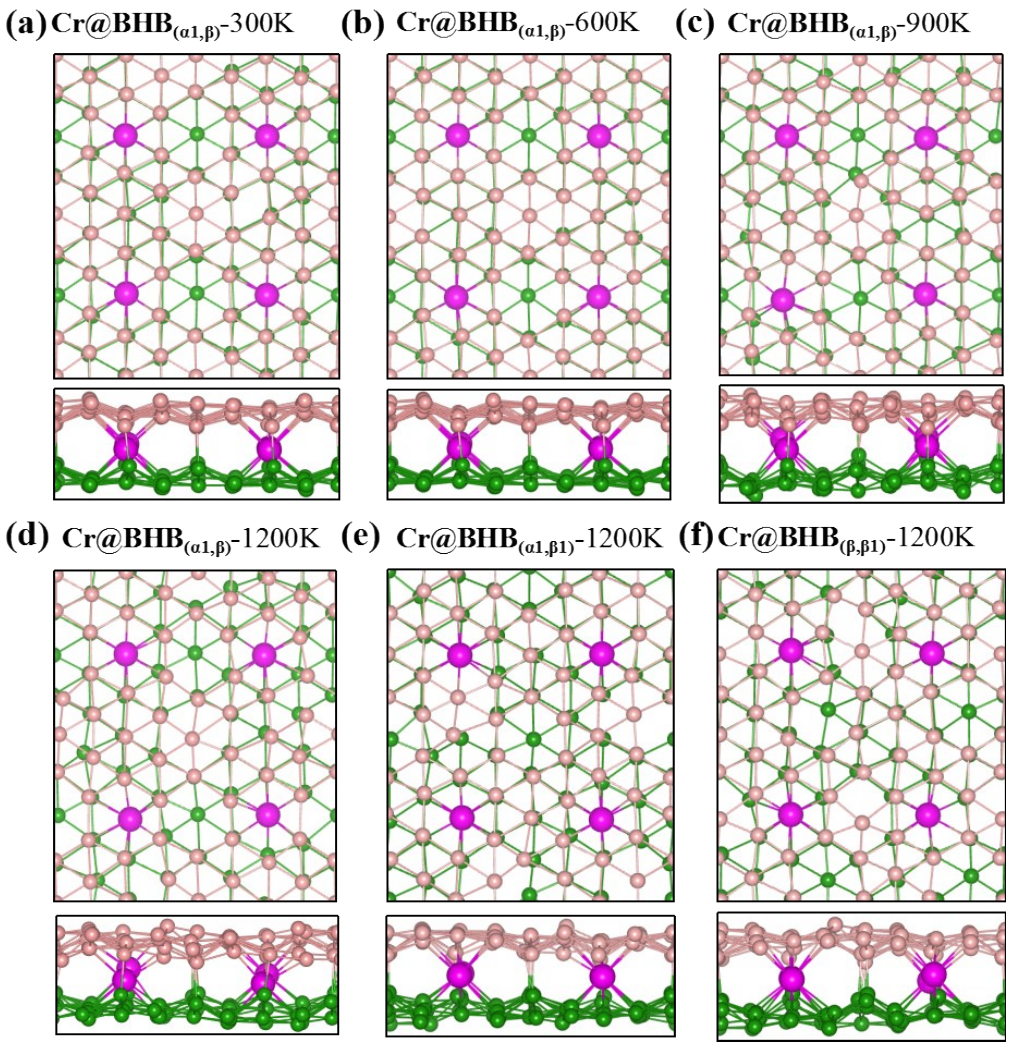

Fig. S2 (a-d) $Cr@BHB_{(\alpha1,\beta)}$ after AIMD simulation at temperature of 300K, 600K, 900K and 1200K, respectively; (e) $Cr@BHB_{(\alpha1,\beta1)}$ after AIMD simulation at temperature of 1200K; (f) $Cr@BHB_{(\beta,\beta1)}$ after AIMD simulation at temperature of 1200K.

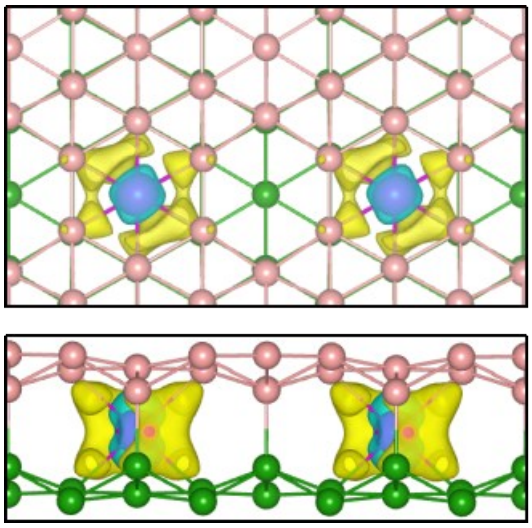

Fig. S3 Charge density differences of Cr@BHB$_{(\alpha1,\beta)}$. Yellow and blue colors indicate charge accumulation and depletion, respectively. The isosurface value was set at 0.01 a.u.

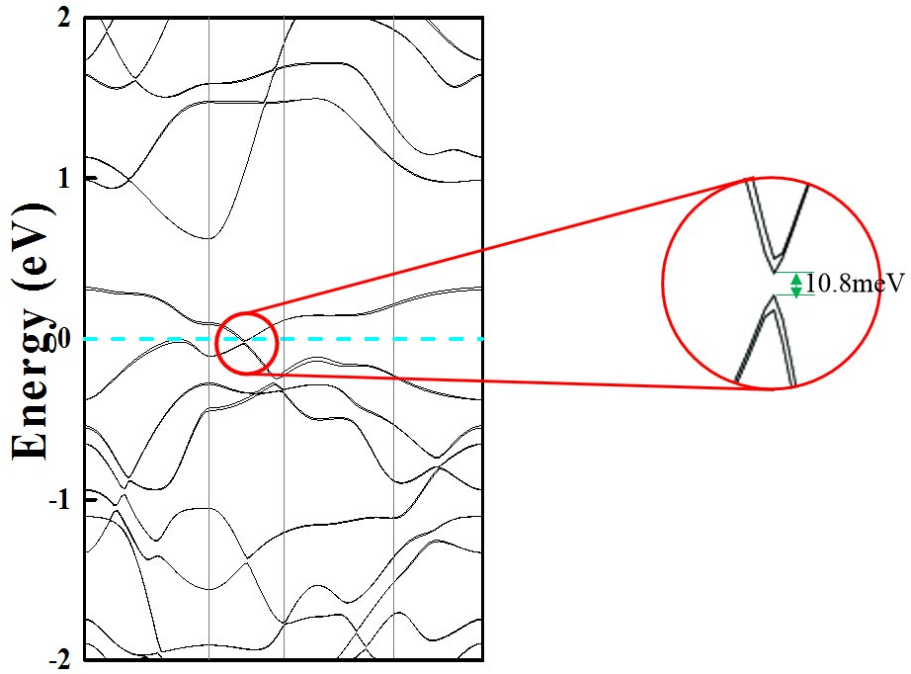

Fig. S4 Spin-orbit splitting of the Dirac point for Cr@BHB$_{(\alpha1,\beta)}$.

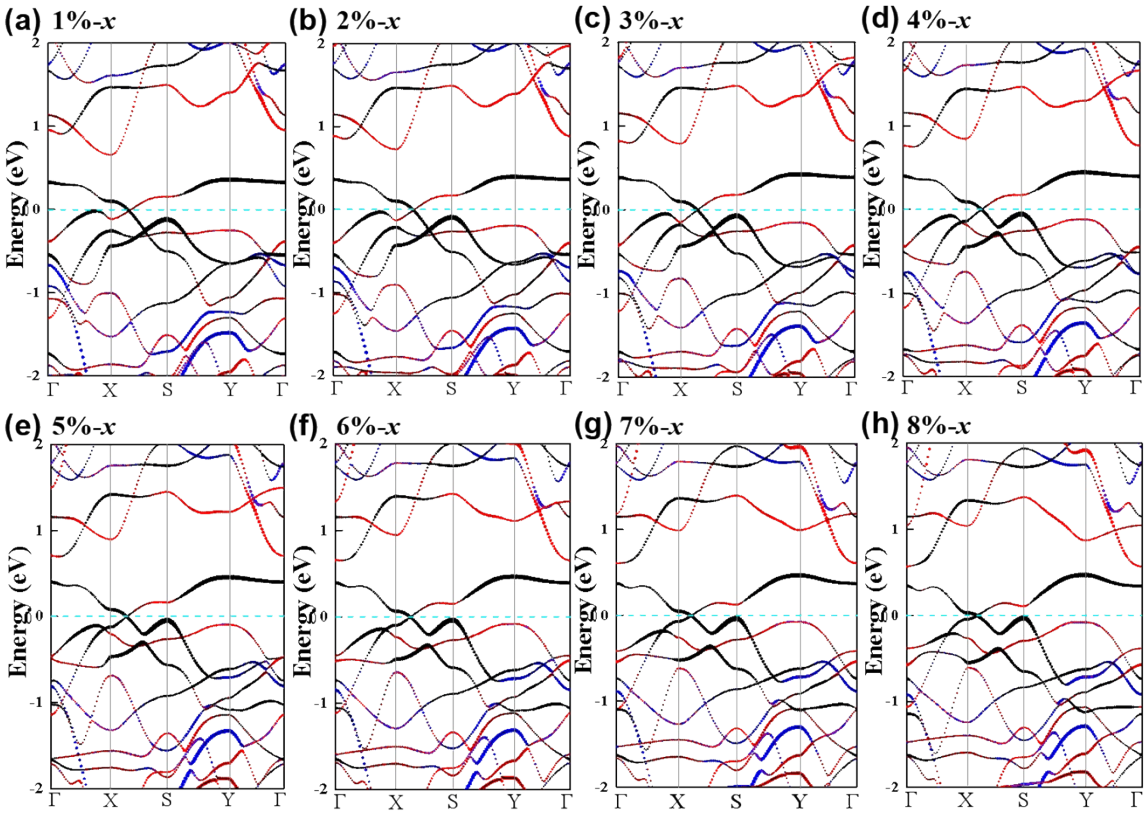

Fig. S5 Band structures of the Cr@BHB$_{(\alpha 1,\beta)}$ under uniaxial tensile strains along *x* direction from 1% to 8%, Dirac state can be preserved up to 8%.

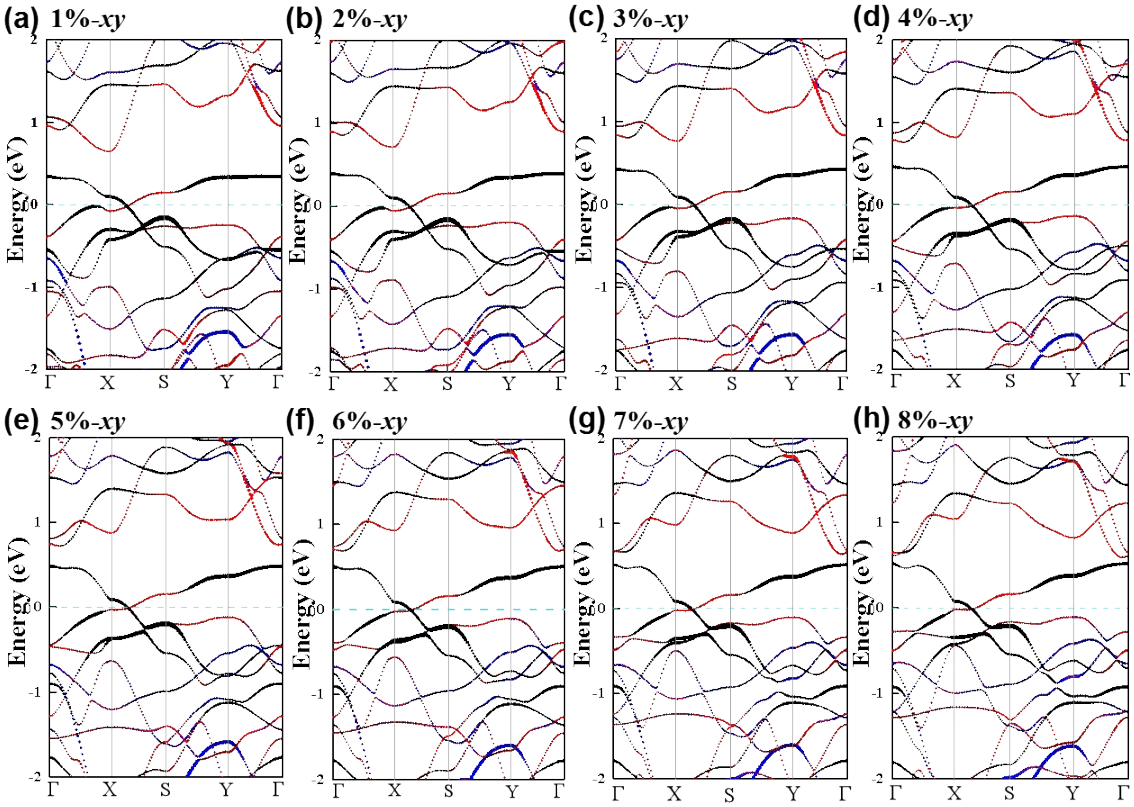

Fig. S6 Band structures of the Cr@BHB$_{(\alpha1,\beta)}$ under biaxial tensile strains along *xy* direction from 1% to 8%, Dirac state can be preserved up to 8%.

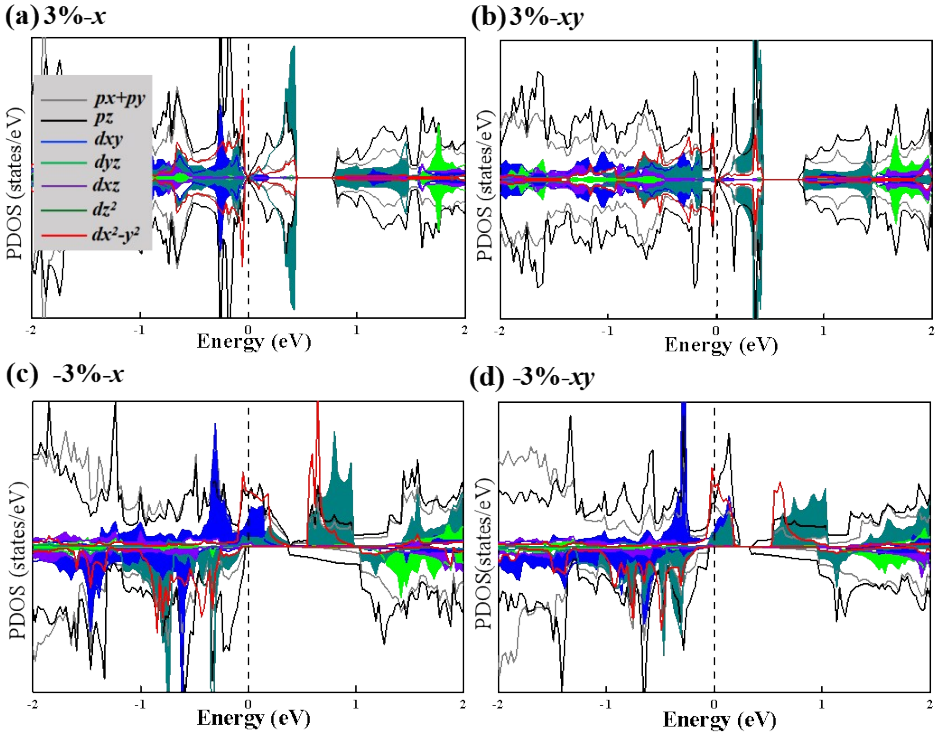

Fig. S7 The partial density of states for Cr@BHB$_{(\alpha1,\beta)}$ under stretch and compressive strain of 3%.

Table S1. The transferred electrons (Δe, e) from Cr atom to BHB for Cr@BHB$_{(\alpha1,\beta)}$ under biaxial strains and uniaxial strains along *x* and *y* directions calculated by bader charge.

	Strain intensity(%)							
Δe	1	2	3	4	5	6	7	8
x	0.74	0.73	0.73	0.73	0.73	0.73	0.73	0.72
y	0.73	0.74	0.75	0.74	0.76	0.78	0.79	0.79
xy	0.73	0.73	0.75	0.75	0.75	0.74	0.75	0.75
	Strain intensity(%)							
Δe	-1	-2	-3	-4	-5	-6	-7	-8
x	0.84	0.85	0.86	0.86	0.86	0.87	0.87	0.88
y	0.82	0.82	0.82	0.81	0.77	0.77	0.76	0.76
xy	0.84	0.84	0.85	0.86	0.86	0.86	0.84	0.86

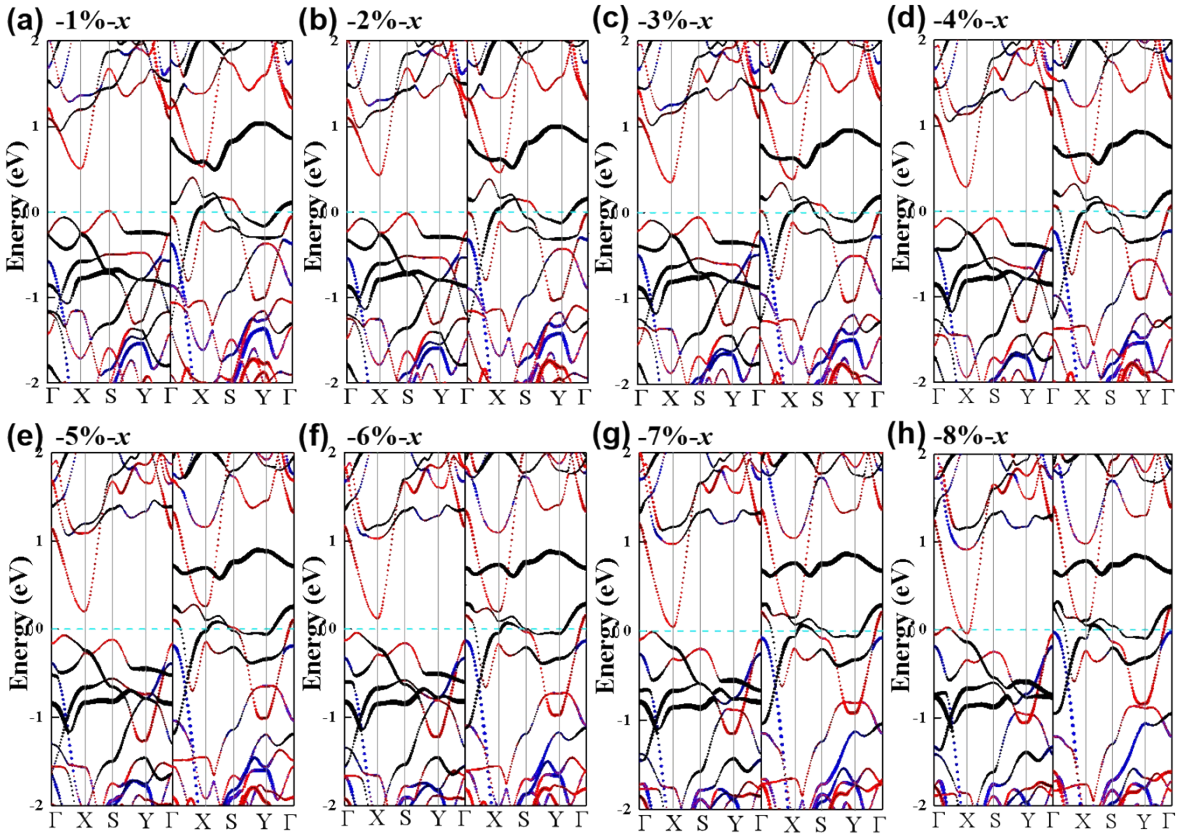

Fig. S8 Band structures of the Cr@BHB$_{(\alpha1,\beta)}$ under uniaxial compressive strains along *x* direction from -1% to -8%.

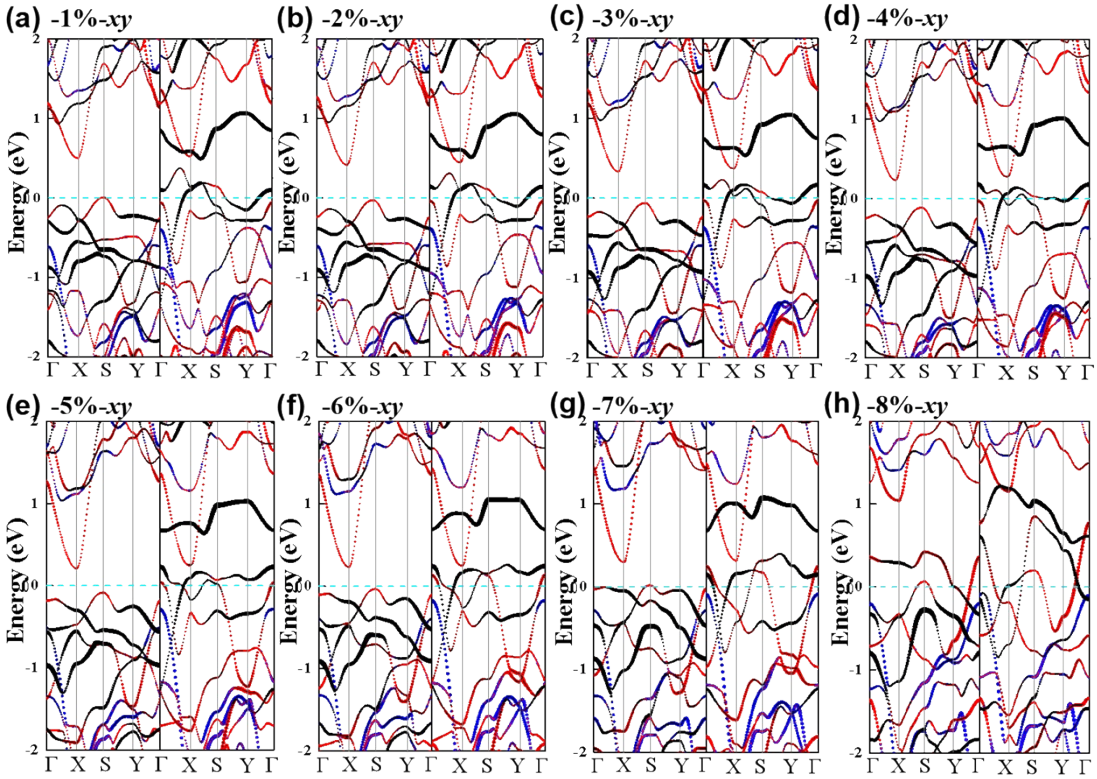

Fig. S9 Band structures of the Cr@BHB$_{(\alpha1,\beta)}$ under biaxial compressive strains from -1% to -8%.

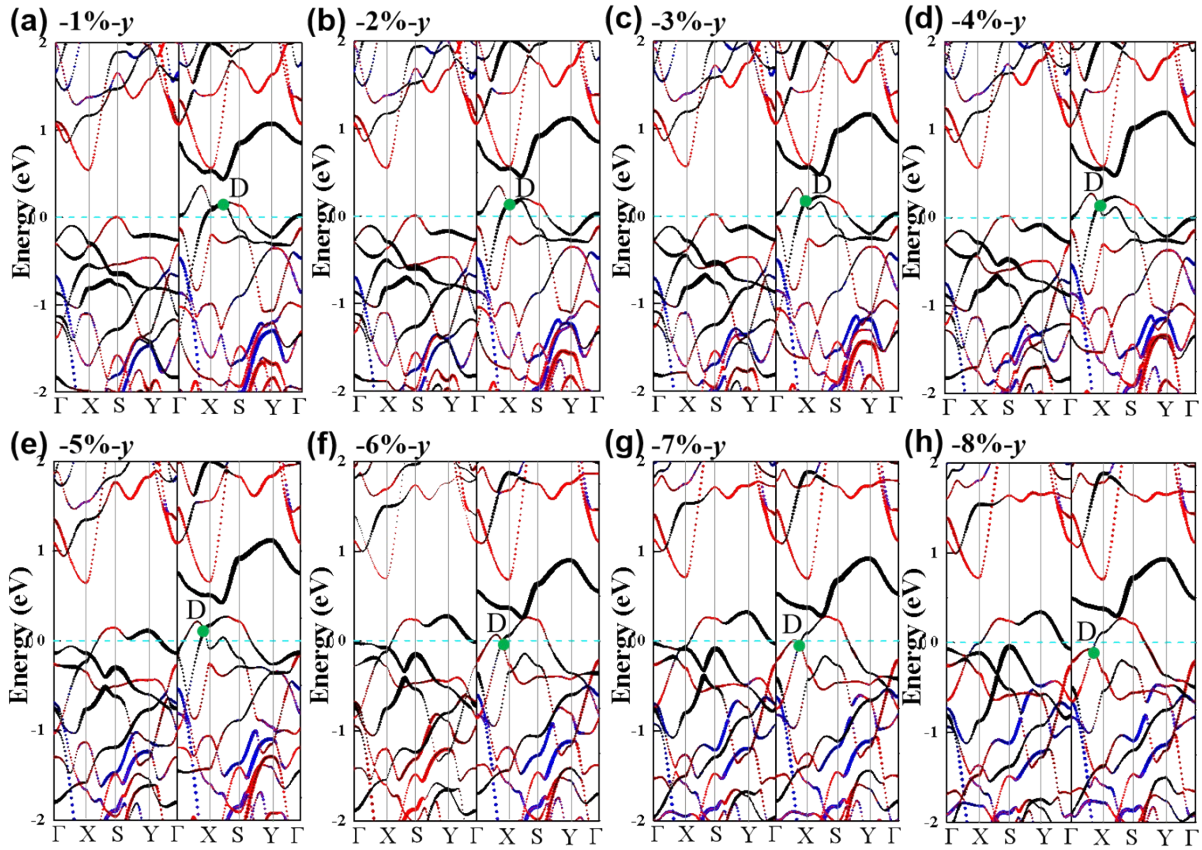

Fig. S10 Band structures of the Cr@BHB$_{(\alpha 1,\beta)}$ under uniaxial compressive strains along *y* direction from -1% to -8%.

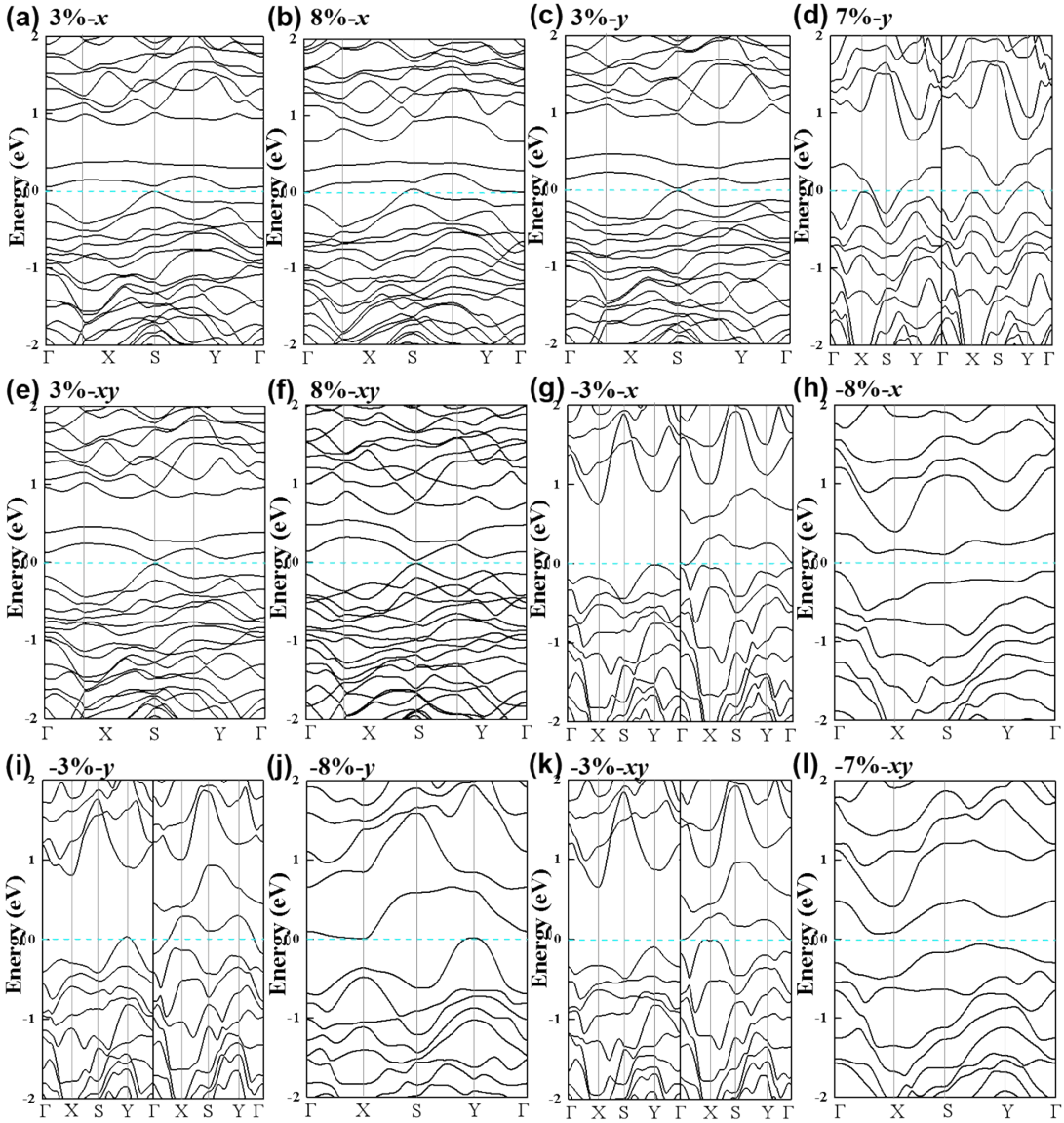

Fig. S11 Band structures of the Cr@BHB$_{(\alpha 1,\beta 1)}$ under different strains.

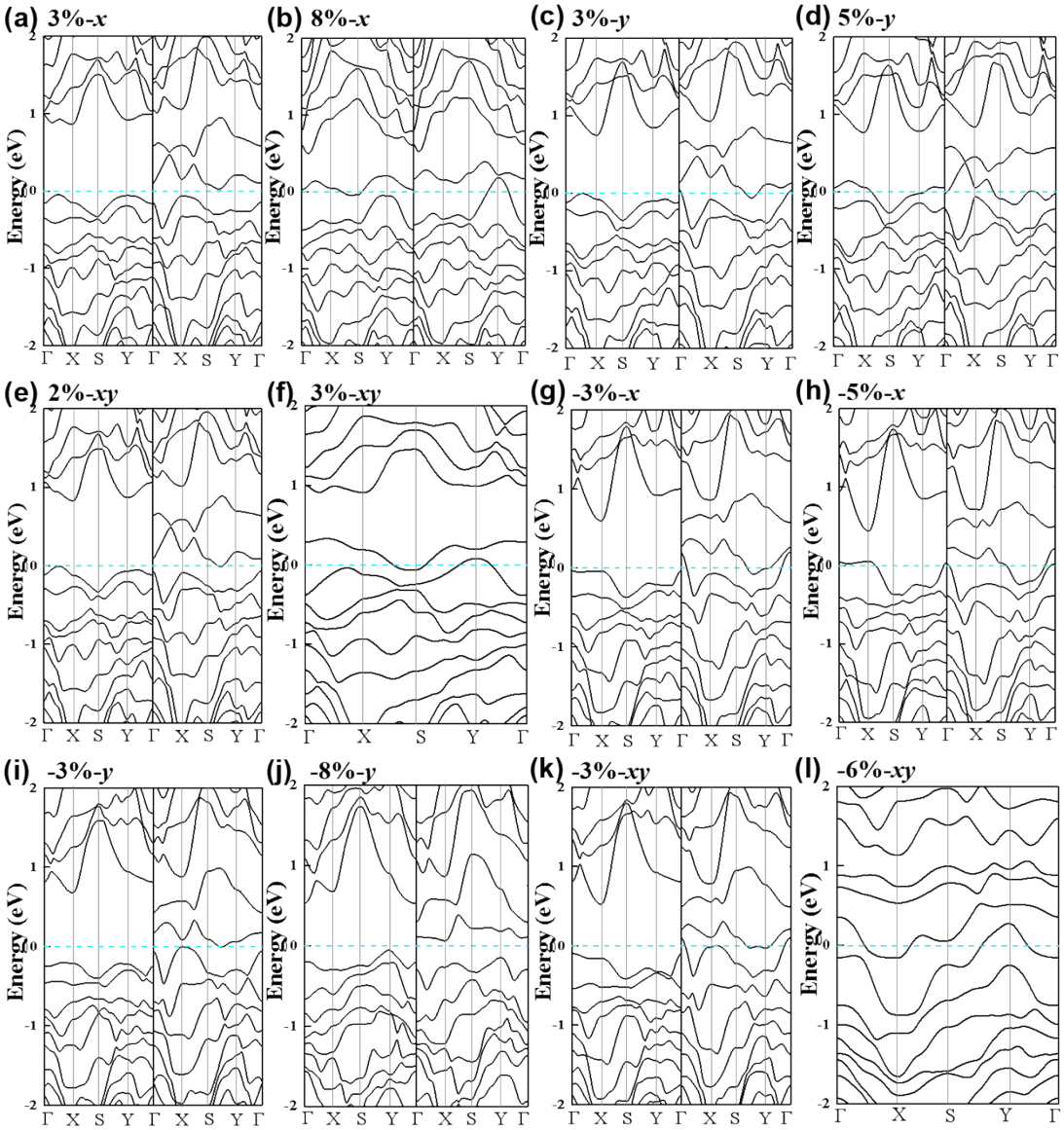

Fig. S12 Band structures of the Cr@BHB$_{(\beta,\beta1)}$ under different strains.

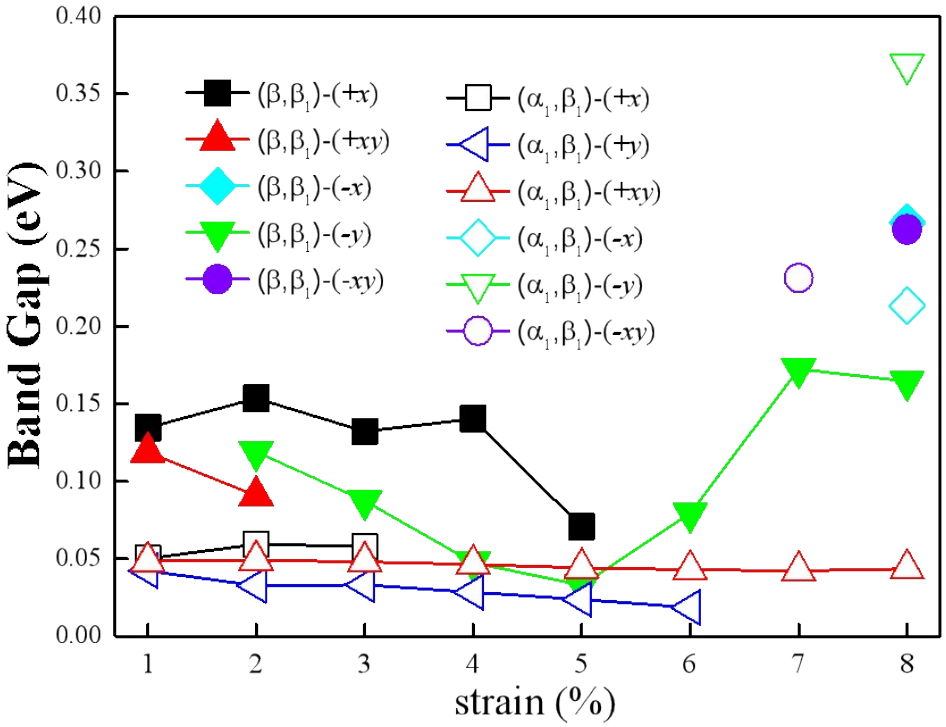

Fig. S13 Band gaps for semiconducting systems of Cr@BHB$_{(\alpha1,\beta1)}$ and Cr@BHB$_{(\beta,\beta1)}$ under strains with different intensities.