Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Table S1 the lattice constant (*a* and *b*) and the average bond length ($d_{Sb\text{-}Sb}$, $d_{Sb\text{-}Bi}$, and $d_{Bi\text{-}Bi}$ denote the bond legth of Sb-Sb, Sb-Bi, and Bi-Bi, respectively) of the antimonene, bismuthene, and Sb_mBi_n LHS

	a (Å)	*b* (Å)	$d_{Sb\text{-}Sb}$ (Å)	$d_{Sb\text{-}Bi}$ (Å)	$d_{Bi\text{-}Bi}$ (Å)
antimonene	4.12	4.12	2.89	-	-
bismuthene	4.32	4.32	-	-	3.04
Sb_2Bi_2	14.65	4.23	2.90	2.97	3.04
Sb_3Bi_3	22.00	4.24	2.90	2.97	3.04
Sb_4Bi_4	29.24	4.24	2.90	2.97	3.04
Sb_5Bi_5	36.53	4.24	2.90	2.97	3.04
Sb_6Bi_6	43.73	4.25	2.90	2.97	3.04
Sb_7Bi_7	51.11	4.24	2.90	2.97	3.04
Sb_8Bi_8	58.35	4.24	2.90	2.96	3.04
Sb_9Bi_9	65.64	4.25	2.90	2.97	3.04
$Sb_{10}Bi_{10}$	72.92	4.24	2.90	2.97	3.04
$Sb_{11}Bi_{11}$	80.29	4.25	2.90	2.97	3.04
$Sb_{15}Bi_{15}$	109.45	4.25	2.90	2.97	3.04
$Sb_{20}Bi_{20}$	152.94	4.25	2.90	2.96	3.04

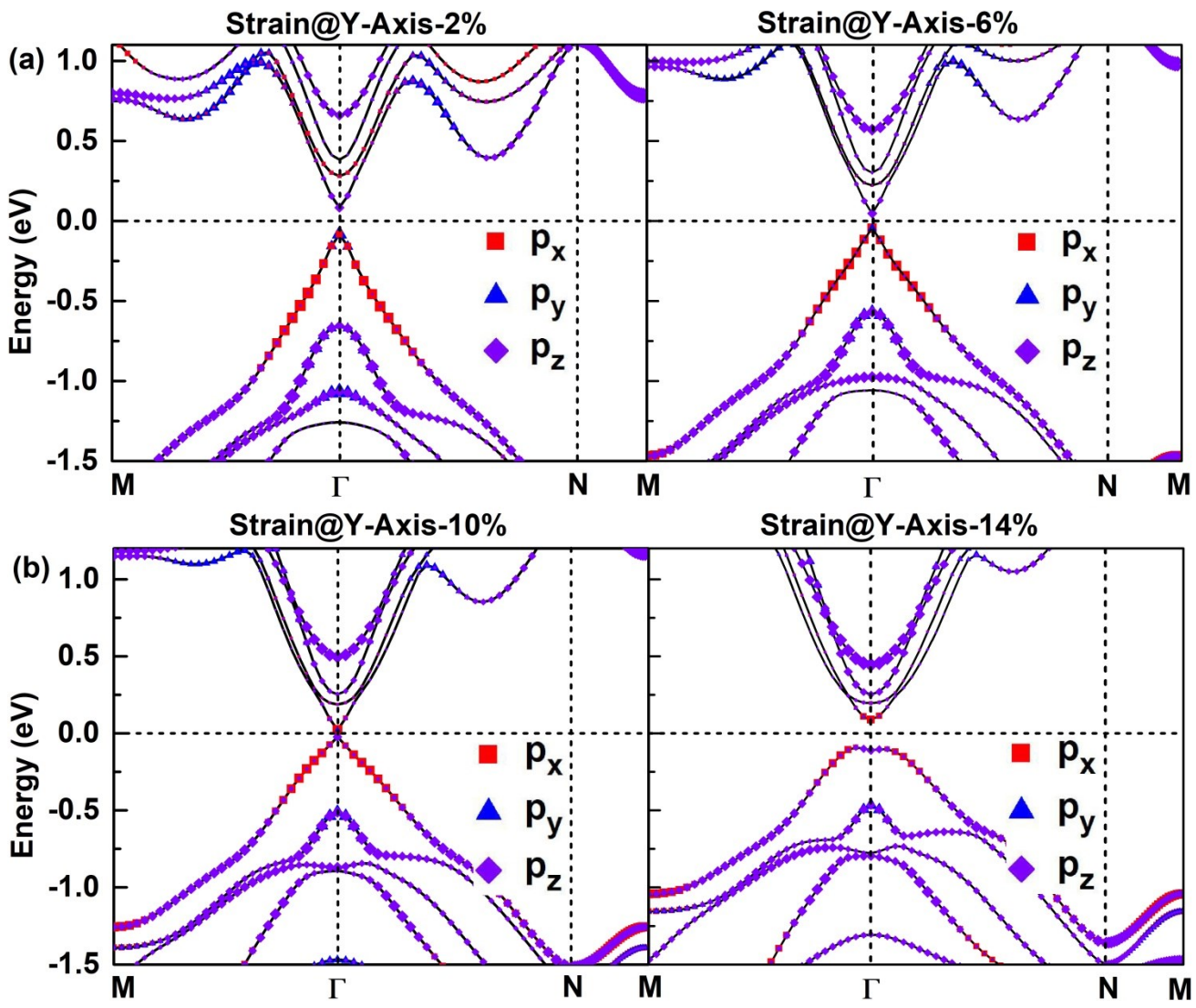

Fig. S1 The orbital-projected bands of strain@Y-axis of Bi atoms of Sb_2Bi_2 LHS. The size of red squares, purple diamonds and blue triangles represent the weights of p_x, p_y, p_z orbitals, respectively.

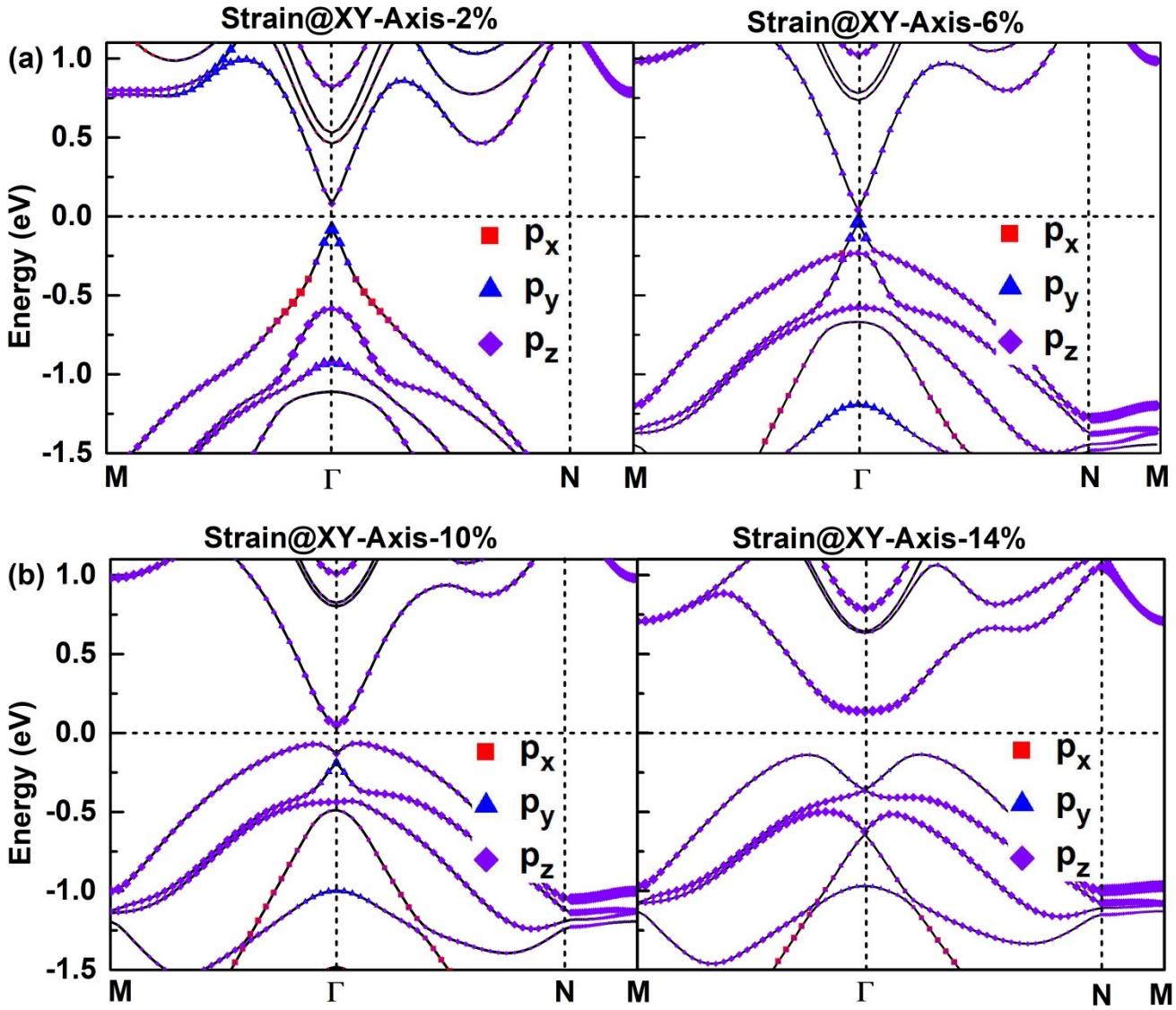

Fig. S2 The orbital-projected bands of strain@XY-axis of Bi atoms of Sb_2Bi_2 LHS. The size of red squares, purple diamonds and blue triangles represent the weights of p_x, p_y, p_z orbitals, respectively.