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Study of Rashba effect in two-dimensional ternary compounds ABC (A = Sb, Bi; B = Se, Te; C = Br; I)

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Supplementary Materials

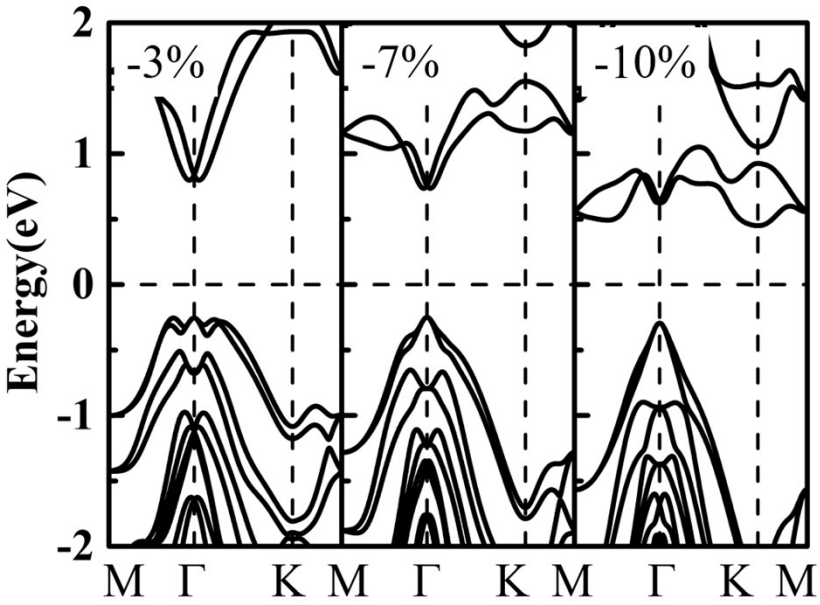

Fig. S1 Energy band structures of BiSeI monolayer with in-plane strains of -3%, -7%, and -10%.

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Table S1 Structural parameters of ABC (A = Sb, Bi; B = Se, Te; C = Br; I) monolayers: space group; lattice constants a; bond length d; bond angle θ; thickness t of monolayer; binding energy E_b.

Systems	*Space group*	*a*(Å)	*d*(Å)		*θ*(°)		*t*(Å)	E_b (eV)
			A-B	*A-C*	*B-A-B*	*B-C-B*		
SbSeI	*P3m1*	4.09	2.80	3.18	93.99	56.39	3.63	-8.26
SbTeI	*P3m1*	4.21	2.98	3.19	90.01	55.79	3.79	-7.90
SbSeBr	*P3m1*	4.01	2.79	3.00	91.88	57.53	3.46	-8.63
SbTeBr	*P3m1*	4.14	2.97	3.01	88.44	57.42	3.59	-8.27
BiSeI	*P3m1*	4.16	2.86	3.25	93.47	55.84	3.74	-8.60
BiTeI	*P3m1*	4.28	3.04	3.26	89.53	55.24	3.90	-8.20
BiSeBr	*P3m1*	4.09	2.85	3.06	91.71	57.36	3.55	-9.00
BiTeBr	*P3m1*	4.22	3.03	3.07	88.22	57.17	3.68	-8.60