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Supporting information

Ideal Strength and Strain Engineering of Rashba Effect in Two-Dimensional BiTeBr

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To verify the stability calculation based on our stress-strain curve, we also carry out the calculations of elastic stiffness constants of BiTeBr monolayers. With the Born-Huang stability criteria as described by

$$C_{11} > 0,\ C_{22} > 0,\ C_{11} > |C_{12}|,\ C_{66} > 0,$$

we find these structures remain stable under the critical strain of 15% as listed in Tab. S1. This is in good agreement with the stress-strain curve in Fig. 2.

Tab. S1. Elastic Stiffness Constants of BiTeBr monolayer under the biaxial strain from 0 to 17%.

Strain(%)	**C_{11}(N/m)**	**C_{12}(N/m)**	**C_{22}(N/m)**	**C_{66}(N/m)**
0	28.612	7.224	28.612	10.694
7	20.727	3.920	20.727	8.403
10	17.569	2.036	17.569	7.767
13	13.545	0.335	13.545	6.605
15	25.418	6.598	25.418	9.410
16	-6.261	12.698	-6.261	-9.480
17	-29.849	32.959	-29.849	-31.404

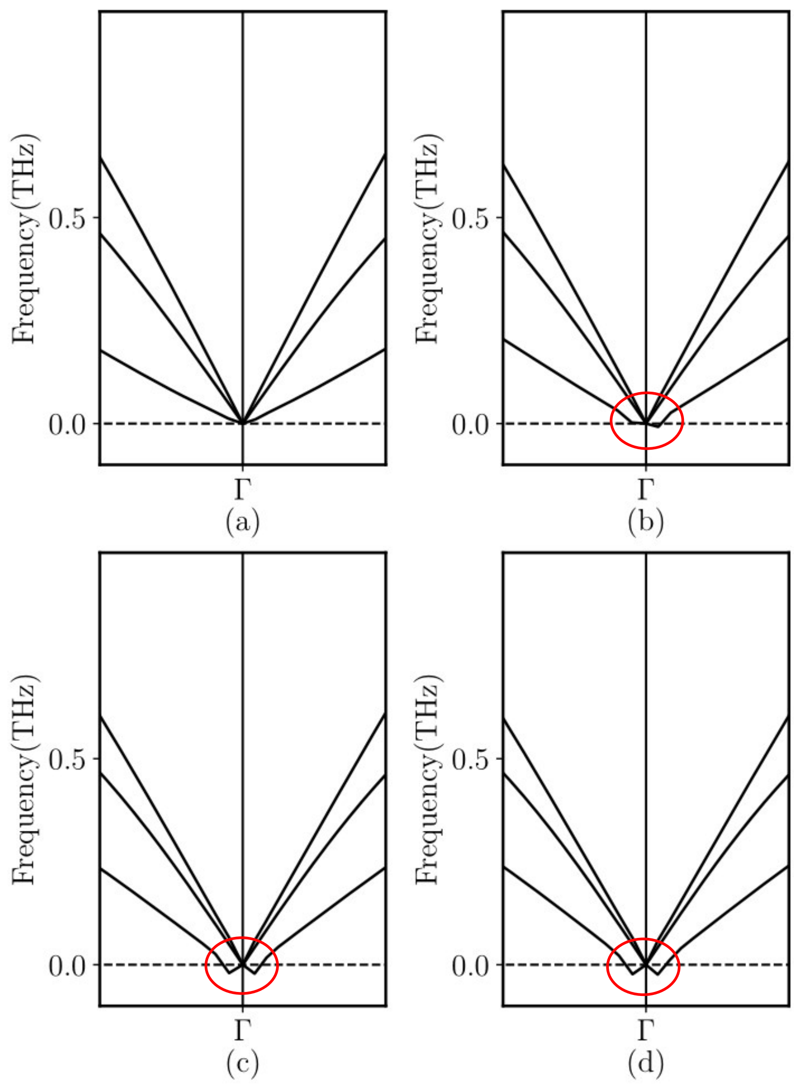

Fig. S1. The small virtual frequencies around Γ point in phonon spectra under a biaxial tensile strain (a) $\varepsilon = 0\%$, (b) $\varepsilon = 3\%$, (c) $\varepsilon = 7\%$ and (d) $\varepsilon = 8\%$.

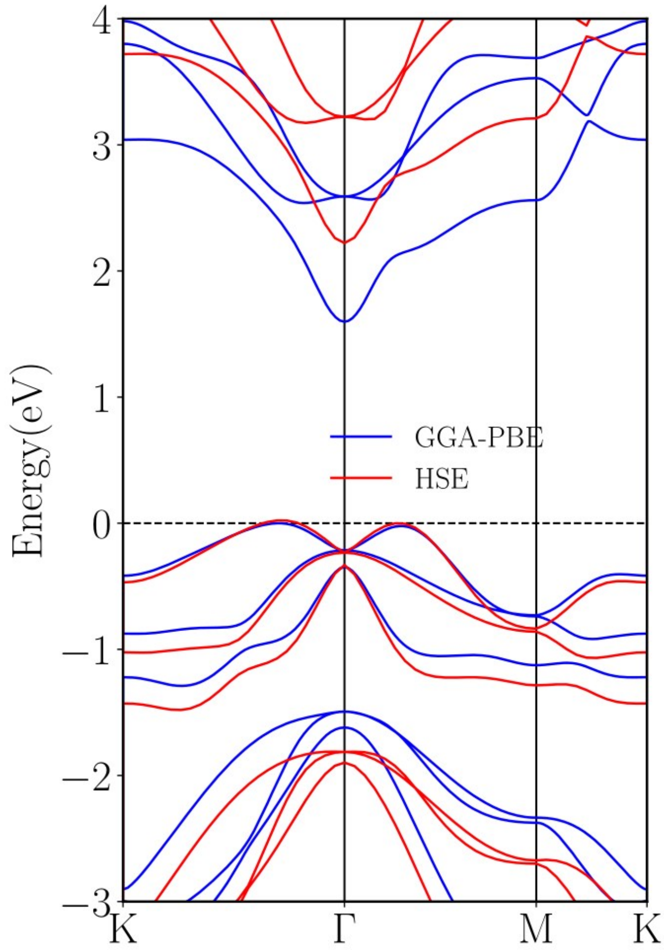

Fig. S2. Electronic band structures calculated using PBE (blue) and HSE06 (red) for a strain-free monolayer without considering spin-orbit coupling.

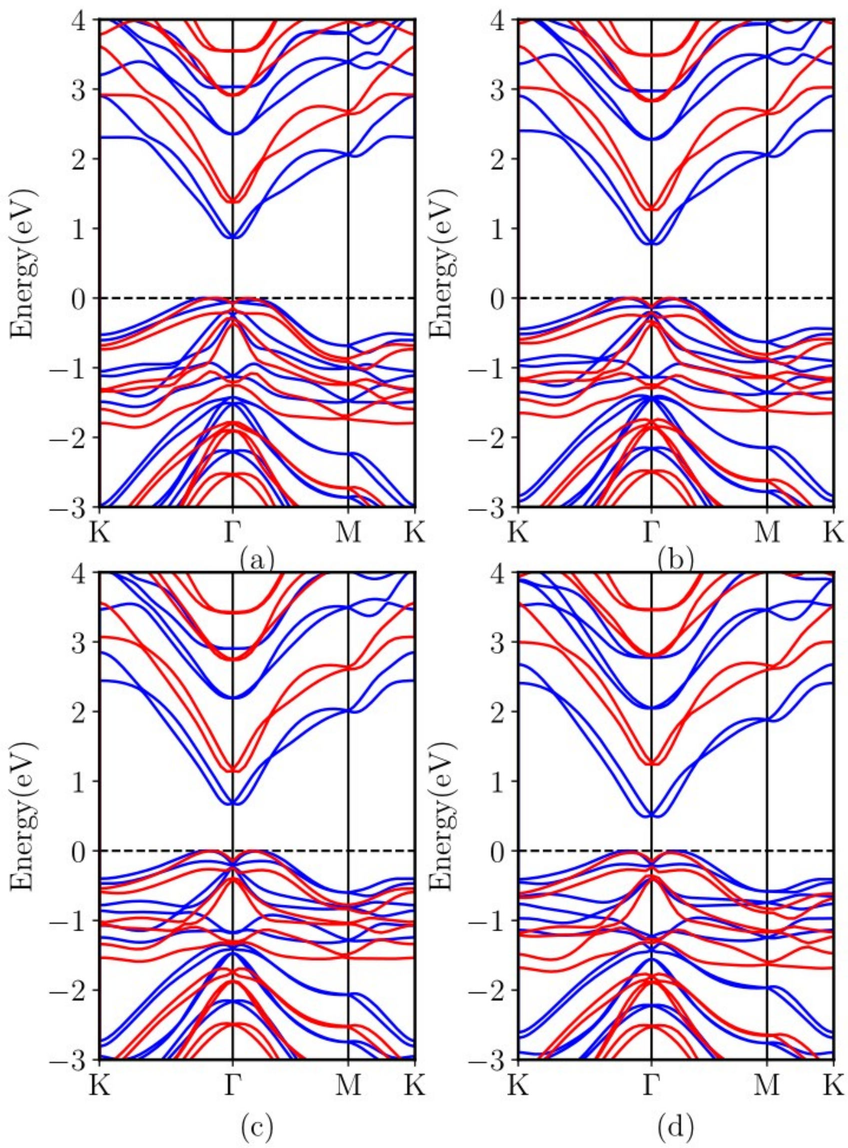

Fig. S3. Electronic band structures of BiTeBr monolayer using PBE (blue) and HSE06 (red) under the applied strain of (a) 0%, (b) 2%, (c) 4% and (d) 7% with spin-orbit coupling included.

Although the BiTeBr monolayer is mechanically stable and dynamically stable when the biaxial tensile strain less than 8%. Here we also present the dependencies of the characteristic parameters of the Rashba spin splitting on the strains in range of 0 to 15% as supplements.

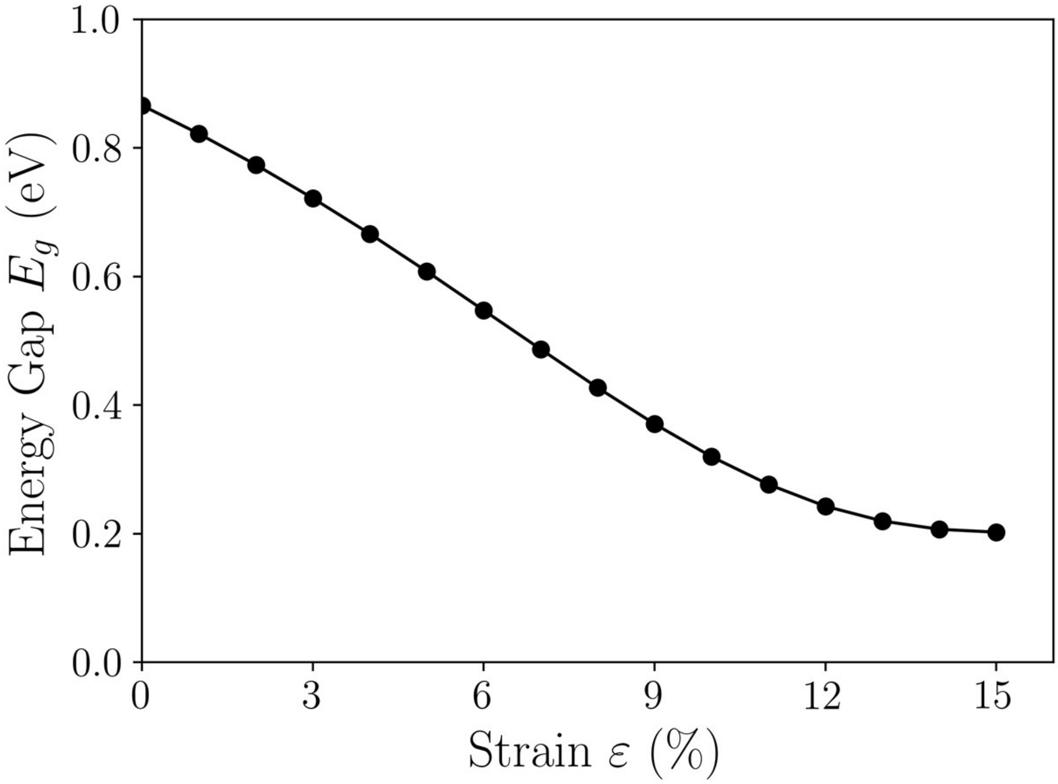

Fig. S4. The PBE energy gap E_g as a function of strain. The band structure demonstrates indirect band gap within the range of all strains.

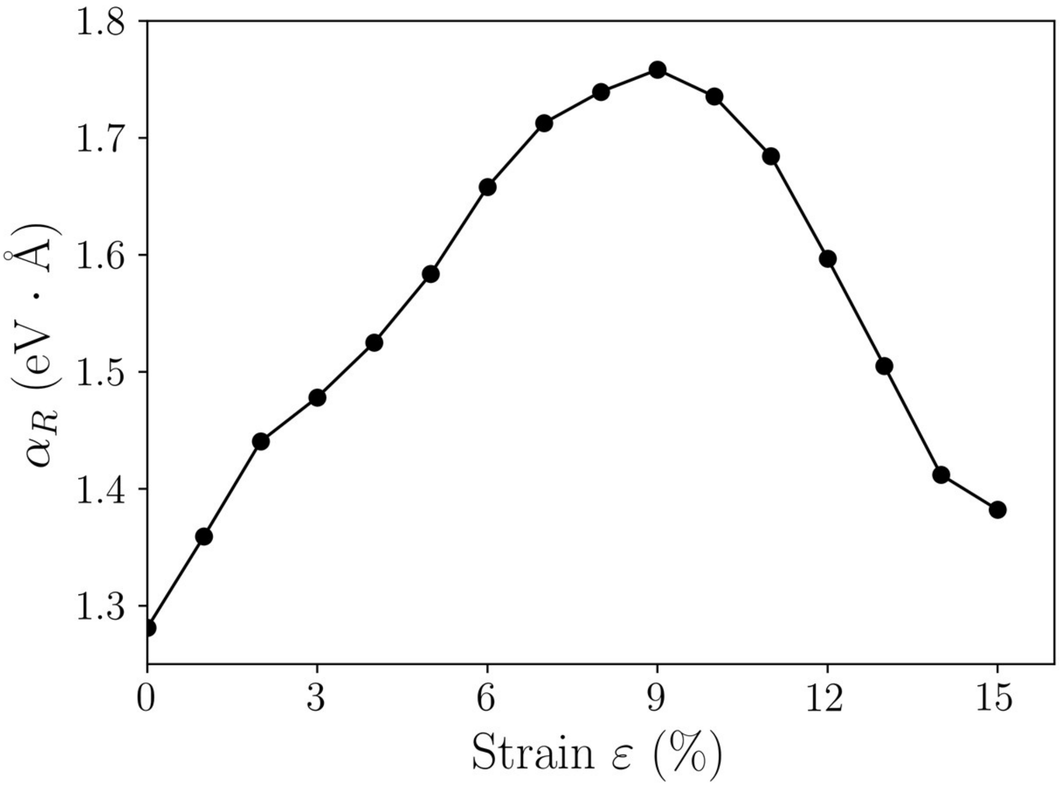

Fig. S5. The PBE Rashba parameter α_R as a function of strain, calculated for the conduction band minimum around the Γ point.

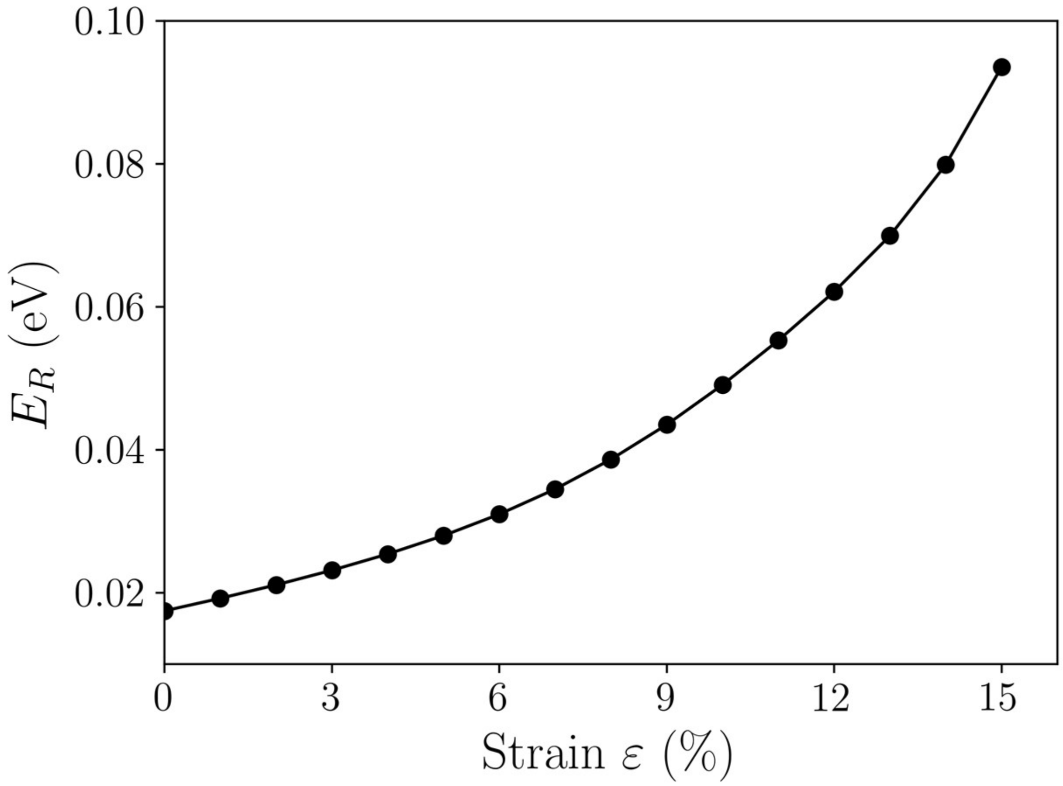

Fig. S6. The PBE Rashba Energy E_R as a function of strain, calculated for the conduction band minimum around the Γ point.

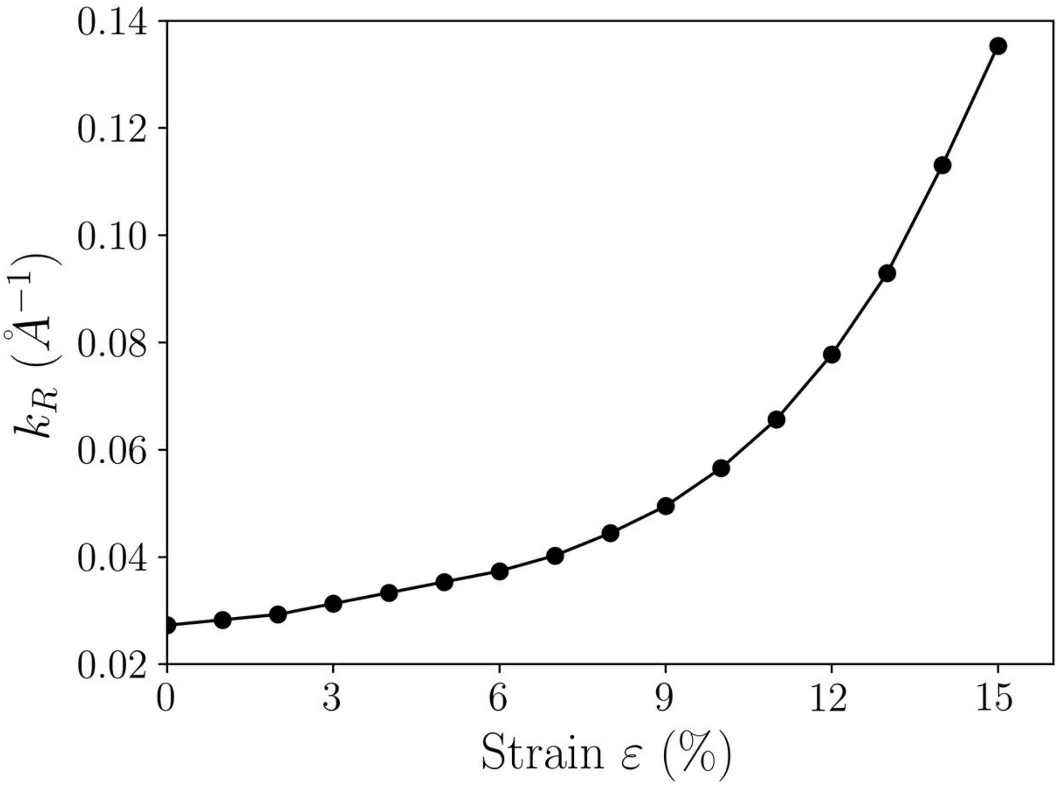

Fig. S7. The PBE momentum offset k_R as a function of strain, calculated for the conduction band minimum around the Γ point.