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Establishing the Correlation between Rashba Spin Splitting and HER Activity Enhancement in Janus Structures

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Notes and references

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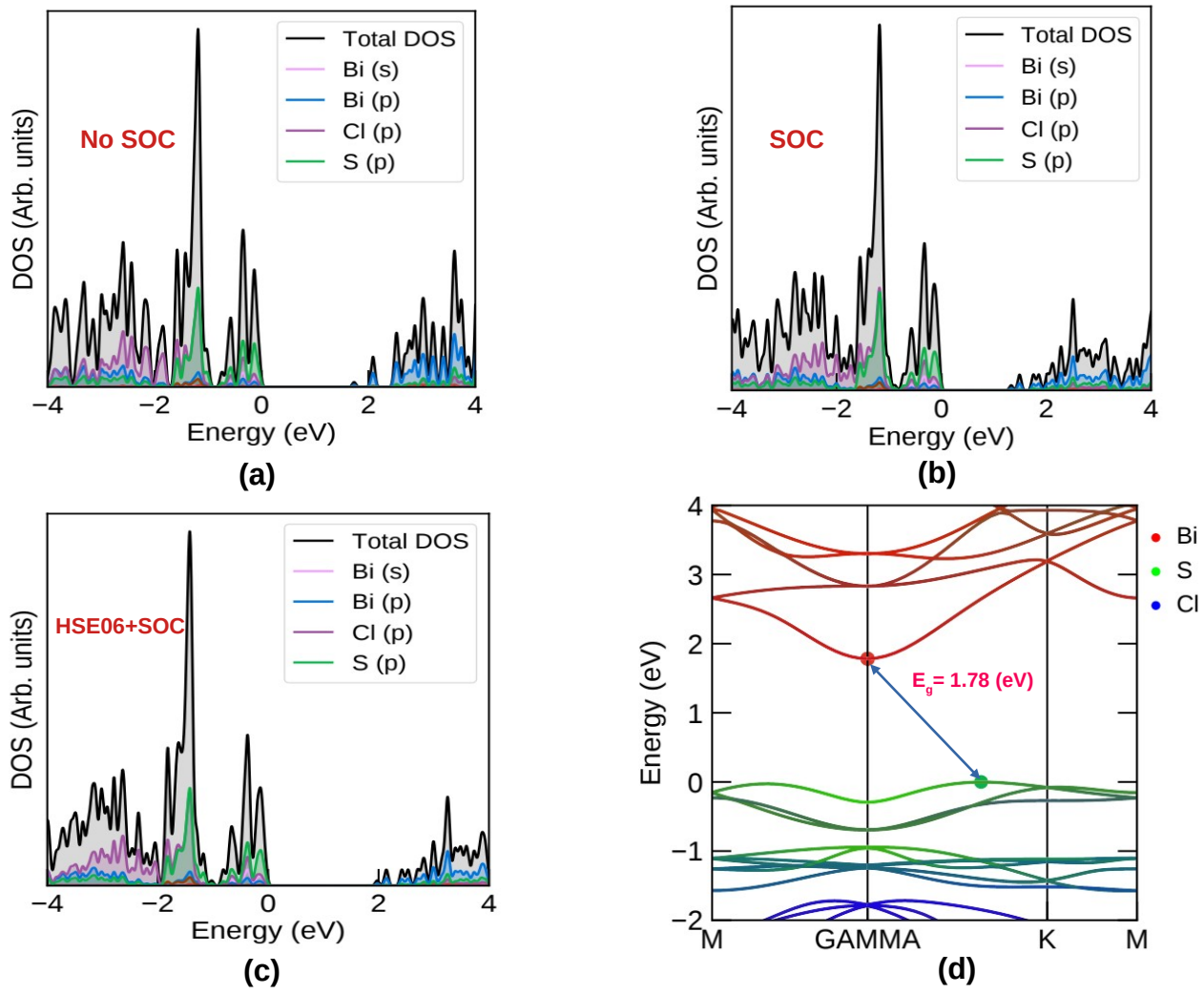

Fig. 1 Total and projected density of states (DOS) of the BiClS monolayer (a) without SOC, (b) with SOC, and (c) with HSE06+SOC. Plot (d) shows the band structure of the Janus BiClS monolayer without the spin-orbit coupling effect.

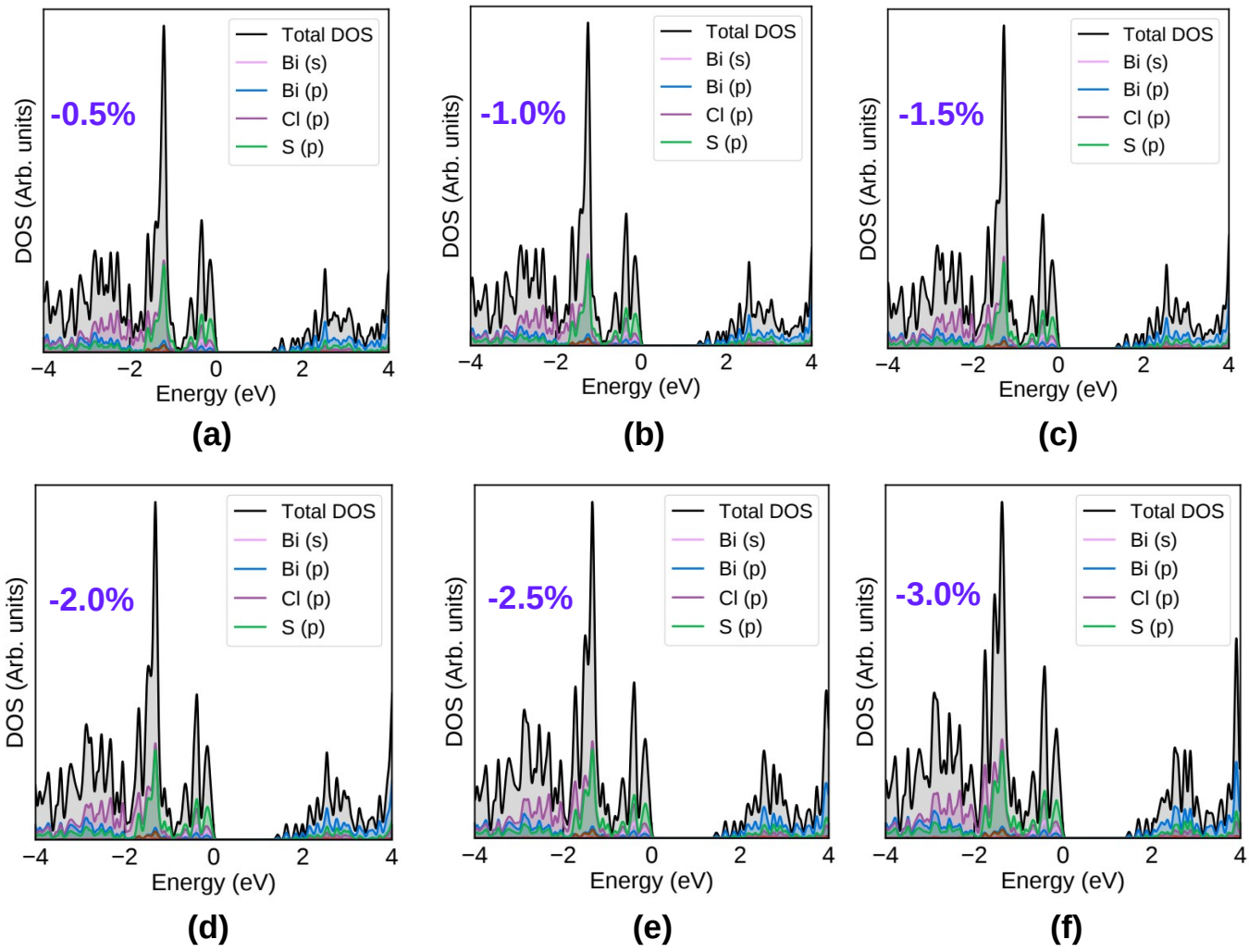

Fig. 2 Total and projected density of states (DOS) of the Janus BiClS monolayer under the compressive strain effect determined by PBE+SOC. Plots (a)-(f) represent the DOS under biaxial compressive strain from 0.5 % to 3.0 % respectively.

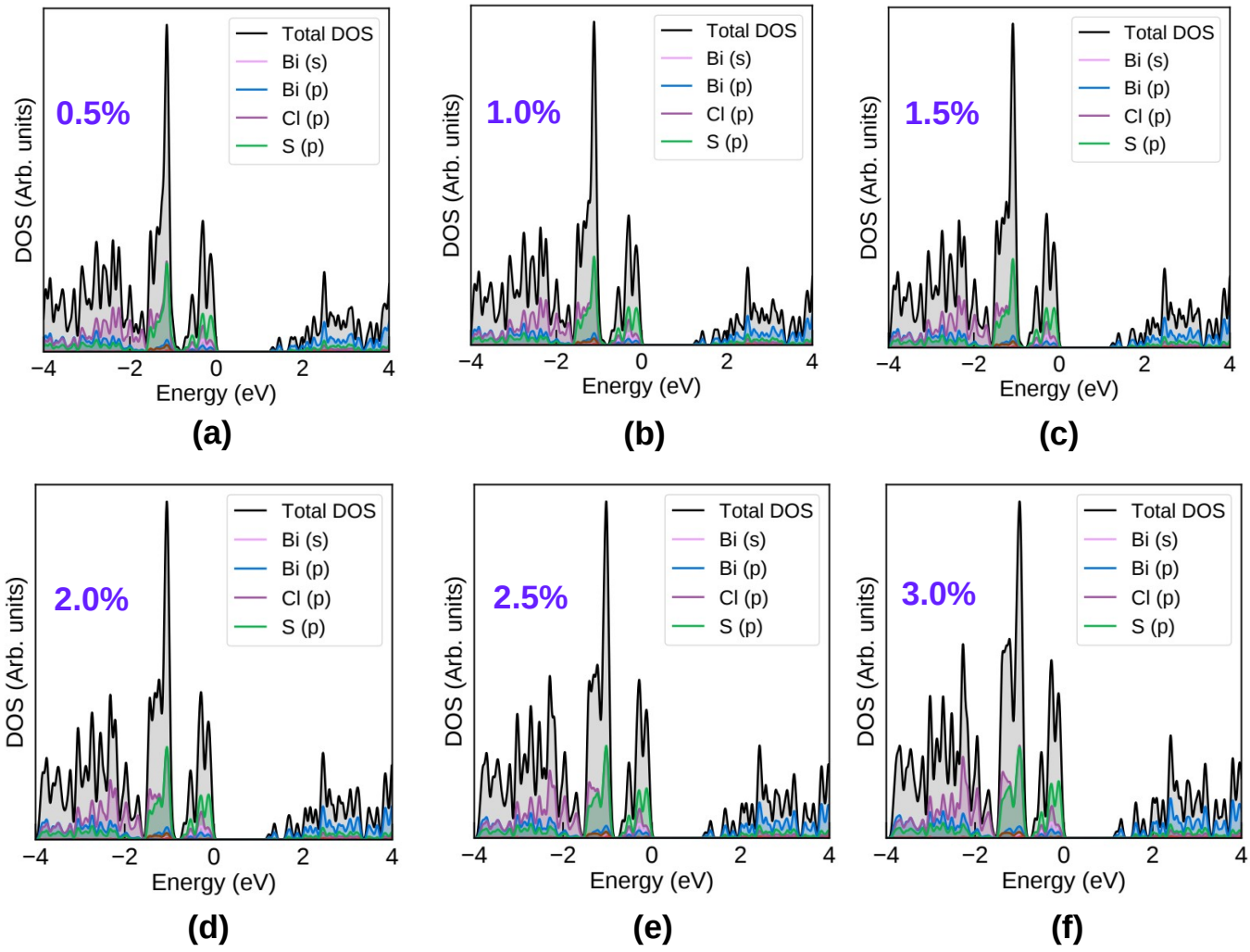

Fig. 3 Total and projected density of states (DOS) of the Janus BiClS monolayer under the tensile strain effect determined by PBE+SOC. Fig. (a)-(f) represent the DOS for tensile strain from 0.5 % to 3.0 % respectively.

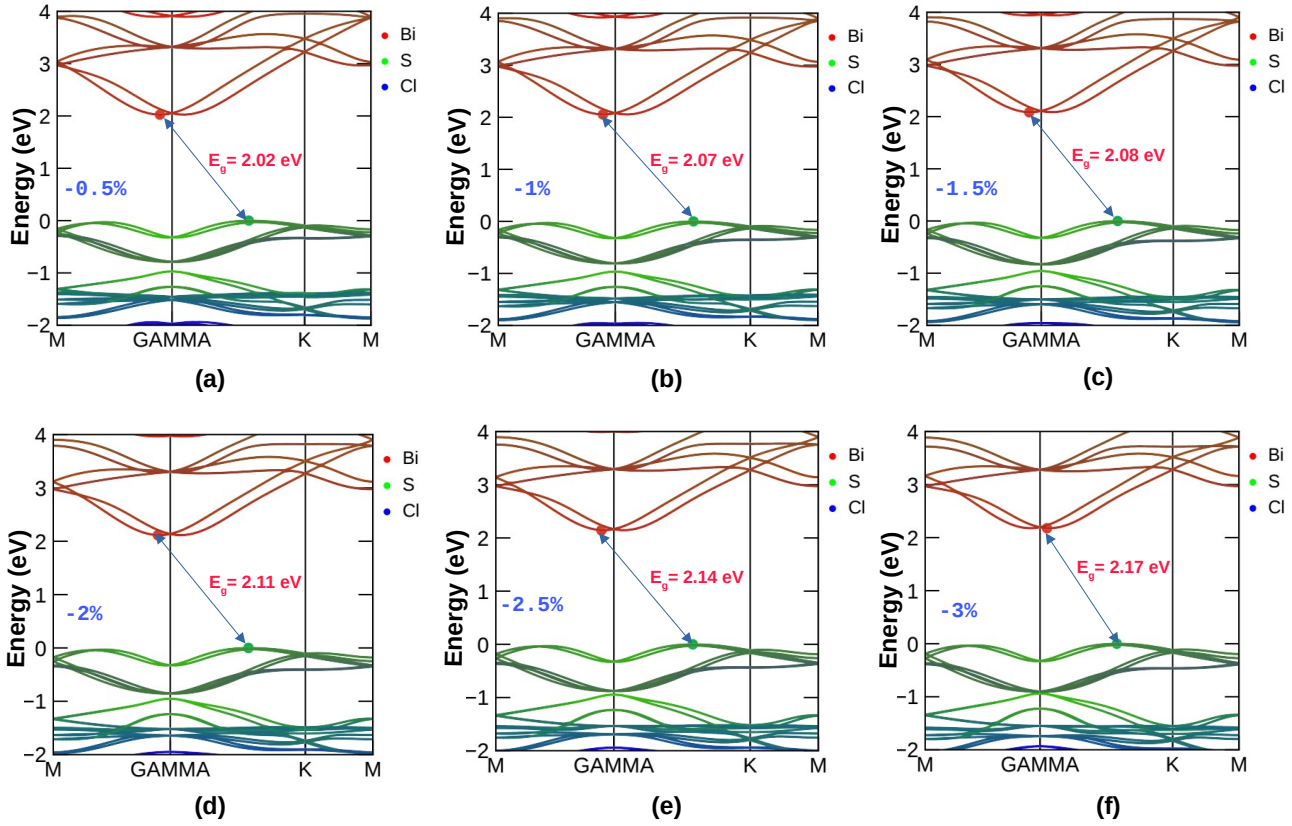

Fig. 4 The band structures of the compressive-strained BiClS monolayer were calculated through HSE06+SOC calculations. From fig. (a) to (f), show the band structure of the monolayer under the compressive strain from $0.5\,\%$ to $3\,\%$. The valence band maxima are set to zero. The values with red (blue) color in all plots represent the bandgap and percentage of applied biaxial strain.

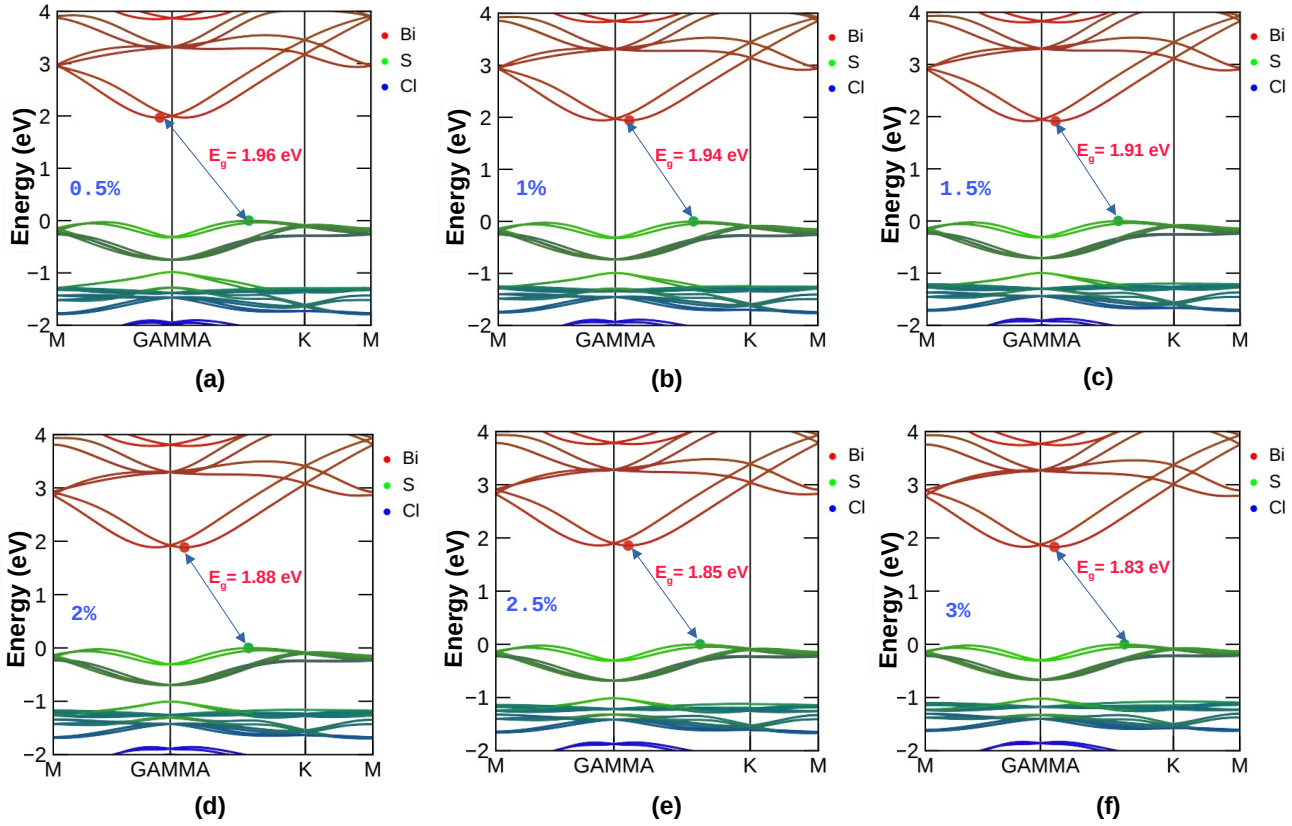

Fig. 5 The band structures of the tensile-strained BiClS monolayer were calculated through HSE06+SOC calculations. From fig. (a) to (f), show the band structure of the monolayer under the tensile strain from 0.5 % to 3 %. The valence band maxima are set to zero. The values with red (blue) color in all plots represent the bandgap and percentage of applied biaxial strain.

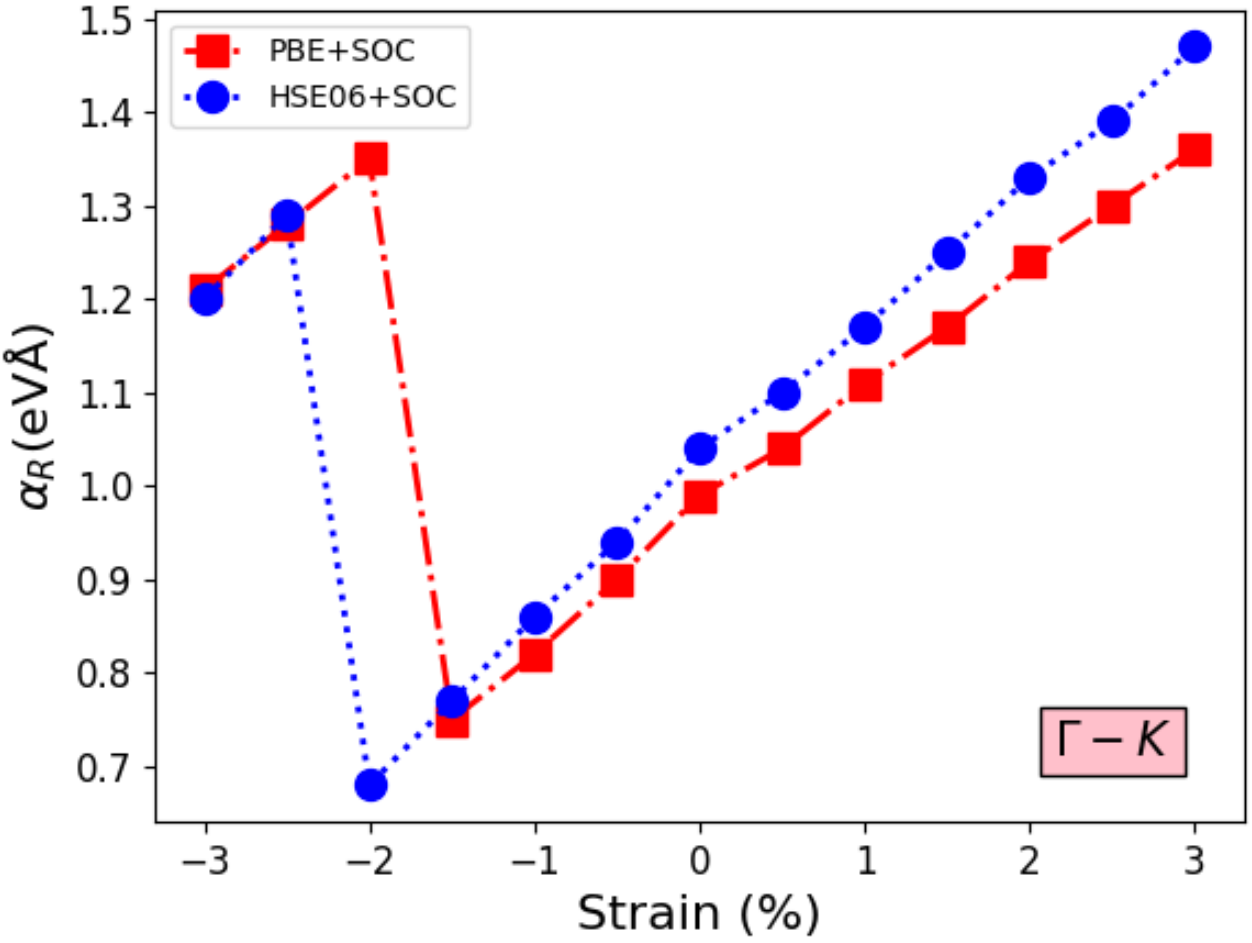

Fig. 6 Rashba spin splitting parameter (α_R) along the direction $\Gamma - K$ obtained from PBE+SOC and HSE06+SOC calculations is plotted as a function of in-plane biaxial strain.

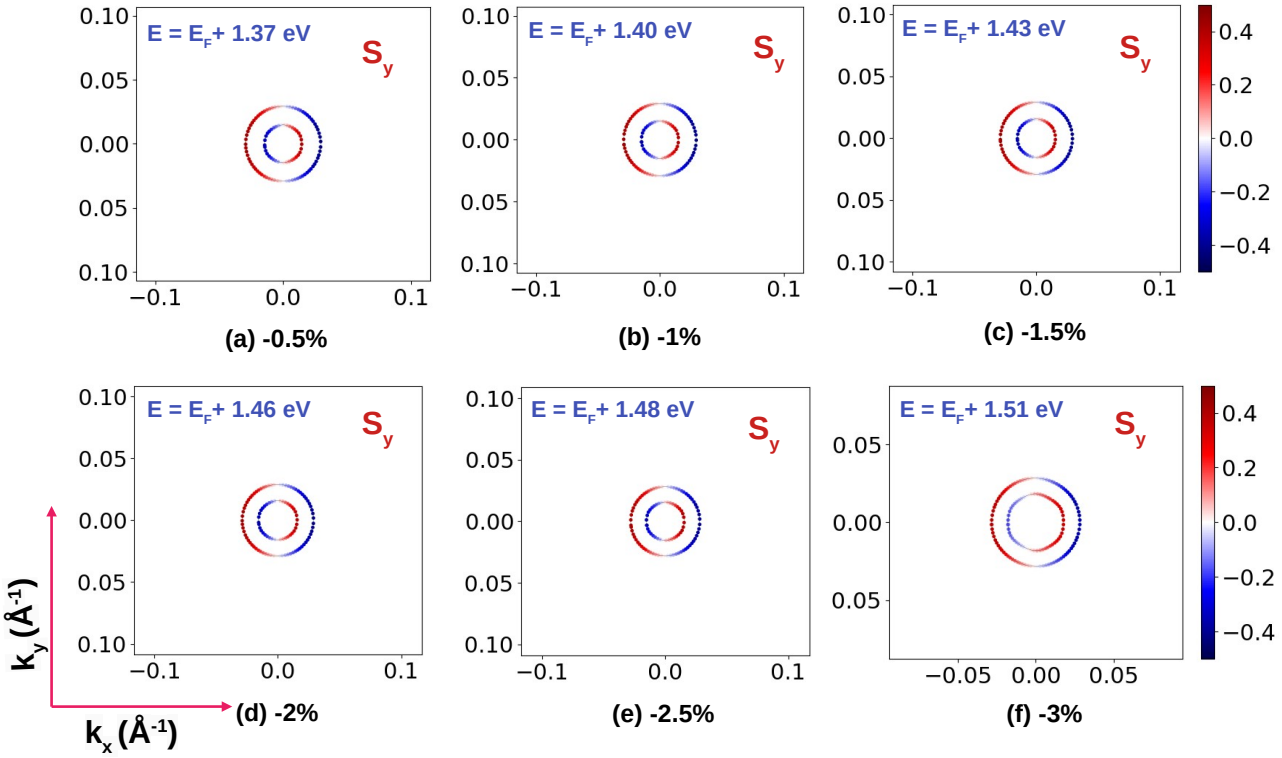

Fig. 7 The S_y projection of spin-texture of the compressive strain-induced Janus BiClS monolayer was calculated from PBE+SOC at constant energy above Fermi level. Plots (a-f) show spin-texture under compressive strain from $0.5\,\%$ to $3\,\%$. The energy above Fermi-level, at which spin texture is plotted, has been written in blue text in all plots

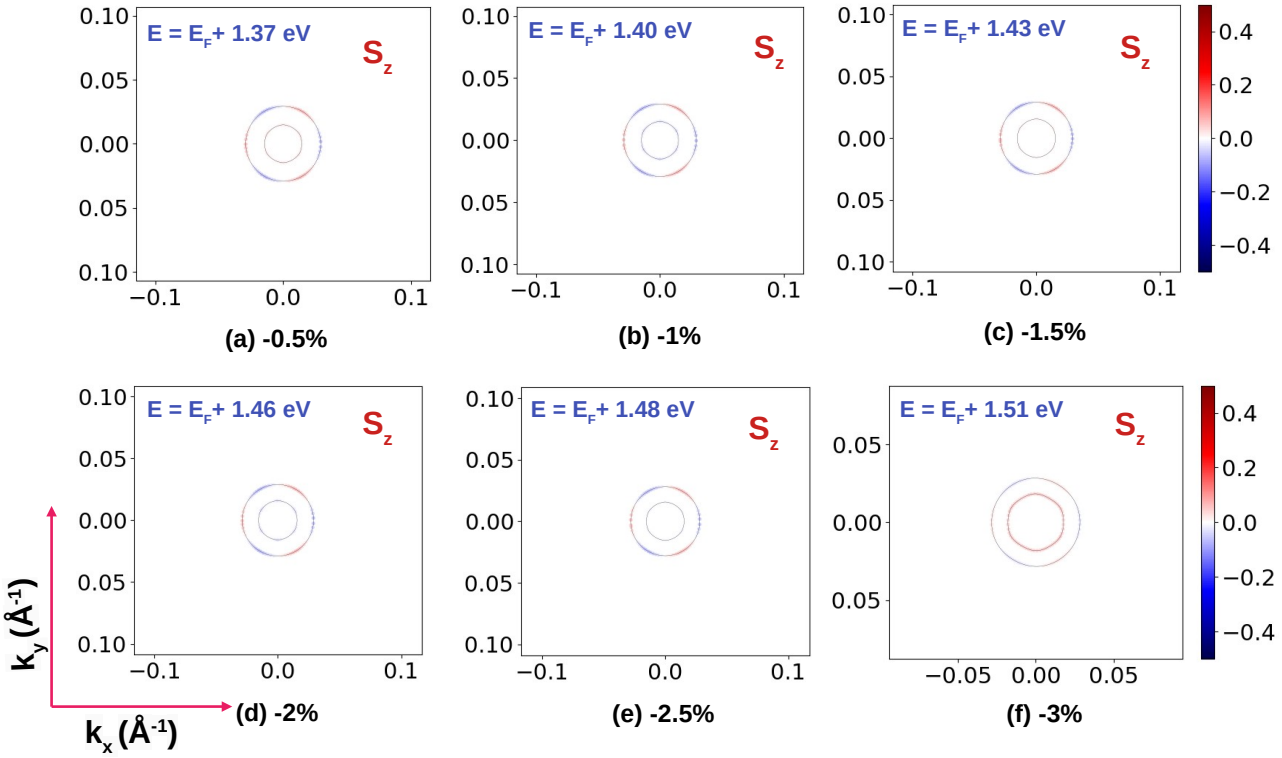

Fig. 8 The S_z projection of spin-texture of the compressive strain-induced Janus BiClS monolayer was calculated from PBE+SOC at constant energy above Fermi level. Plots (a-f) show spin-texture under compressive strain from $0.5\,\%$ to $3\,\%$. The energy above Fermi-level, at which spin texture is plotted, has been written in blue text in all plots.

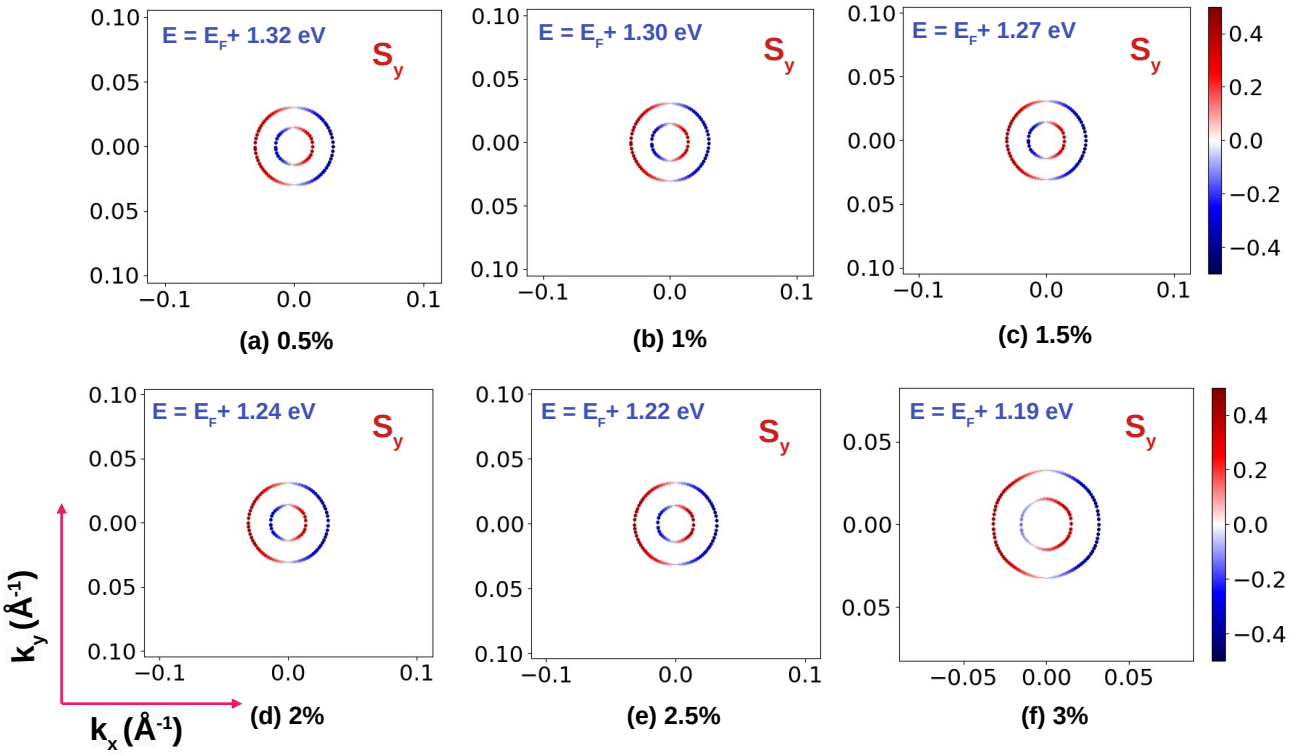

Fig. 9 The S_y spin-texture of the tensile strain-induced Janus BiClS monolayer was calculated from PBE+SOC at constant energy above Fermi level. Plots (a-f) show spin-texture under tensile strain from $0.5\,\%$ to $3\,\%$. The energy above Fermi-level, at which spin texture is plotted, has been written in blue text in all plots.

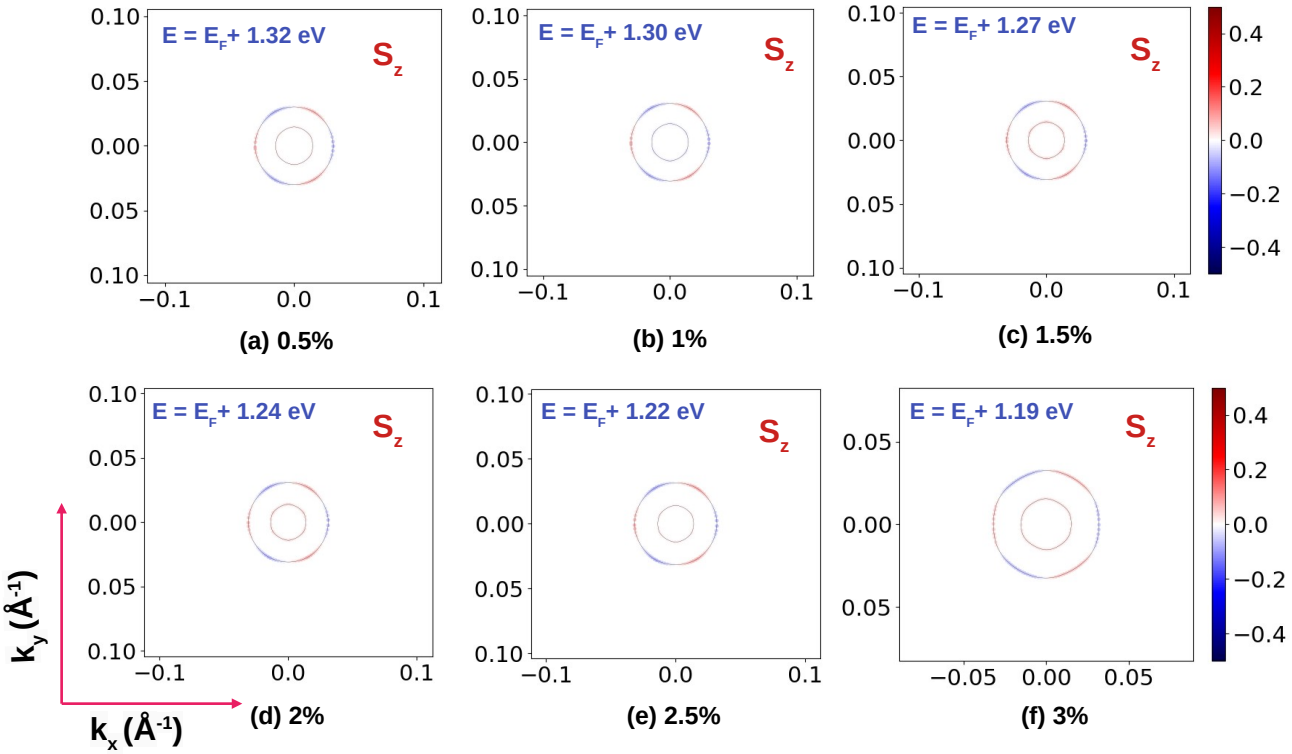

Fig. 10 The S_z spin-texture of the tensile strain-induced Janus BiClS monolayer was calculated from PBE+SOC at constant energy above Fermi level. Plots (a-f) show spin-texture under tensile strain from $0.5\,\%$ to $3\,\%$. The energy above Fermi-level, at which spin texture is plotted, has been written in blue text in all plots.

Table 1 The Rashba energy and momentum offset are obtained from PBE+SOC and HSE06+SOC calculations along the directions of Γ-M and Γ-K, respectively. The negative and positive values in the strain column represent the compressive and tensile strains, respectively.

	PBE+SOC				HSE06+SOC			
	Γ-M		Γ-K		Γ-M		Γ-K	
Strain (%)	E_R (eV)	k_R (Å^{-1})	E_R (eV)	k_R (Å^{-1})	E_R (eV)	k_R (Å^{-1})	E_R (eV)	k_R (Å^{-1})
-0.5	0.0255	0.0471	0.0246	0.0544	0.0265	0.0471	0.0257	0.0544
-1.0	0.0239	0.0474	0.0227	0.0547	0.0248	0.0474	0.0236	0.0547
-1.5	0.0223	0.0476	0.0207	0.0550	0.0229	0.0476	0.0213	0.0550
-2.0	0.0205	0.0478	0.0187	0.0276	0.0209	0.0478	0.0189	0.0553
-2.5	0.0188	0.0481	0.0178	0.0277	0.0189	0.0481	0.0180	0.0277
-3.0	0.0170	0.0483	0.0169	0.0279	0.0168	0.0483	0.0169	0.0279
0.0	0.0274	0.0469	0.0269	0.0541	0.0287	0.0469	0.0283	0.0541
0.5	0.0285	0.0467	0.0283	0.0539	0.0293	0.0467	0.0299	0.0539
1.0	0.0298	0.0464	0.0298	0.0536	0.0315	0.0464	0.0316	0.0536
1.5	0.0311	0.0462	0.0314	0.0533	0.0331	0.0462	0.0336	0.0533
2.0	0.0325	0.0460	0.0332	0.0531	0.0346	0.0460	0.0355	0.0531
2.5	0.0336	0.0457	0.0345	0.0528	0.0359	0.0457	0.0370	0.0528
3.0	0.0347	0.0455	0.0360	0.0526	0.0377	0.0683	0.0388	0.0526

Table 2 DFT+SOC calculated adsorption energy and adsorption free energy of the H adsorbed atom on top of the S atom in the Janus BiClS monolayer.

Strain (%)	Adsorption energy, E_{ads} (eV)	Adsorption Free energy, ΔG_H (eV)
-0.5	0.97	1.21
-1.0	1.02	1.26
-1.5	1.06	1.30
-2.0	1.08	1.32
-2.5	1.10	1.34
-3.0	1.11	1.35
0.0	0.91	1.15
0.5	0.85	1.09
1.0	0.78	1.02
1.5	0.72	0.96
2.0	0.65	0.89
2.5	0.57	0.81
3.0	0.52	0.76