Supplementary Information

Mechanism of mechanically induced topological optoelectronic and spintronic phase transitions in 1D graphene spirals: insight into the role of interlayer coupling

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GSs	Equilibrium Lattice (Å)	Metal-Semiconductor strain τ	PBE (a=5Å) Band-gap(eV)	HSE06(a=5Å) Band-gap(eV)	Spin-polarization	Indirect-direct
S(0,0)	3.42	-0.14	1.79	2.46	no	no
S(1,1)	3.35	0.24	0.23	1.21	yes	no
S(2,1)	3.44	-0.04	1.14	1.70	no	yes
S(2,2)	3.29	0.20	0.39	1.41	yes	no
S(2,3)	3.30	0.12	0.01	0.05	no	yes
S(3,1)	3.38	0.19	0.38	1.38	yes	no
S(3,2)	3.39	0.24	0.10	1.13	yes	no
S(3,3)	3.24	0.19	0.53	1.65	yes	no
S(4,1)	3.33	0.15	0.38	1.42	yes	no
S(4,2)	3.48	-0.07	0.88	1.39	no	yes
S(4,3)	3.34	0.06	0.37	0.69	no	yes
S(5,1)	3.40	0.15	0.24	1.24	yes	no
S(6,1)	3.50	-0.05	0.66	1.12	no	yes

Table S1 Summary of equilibrium lattice (a_0), metal-semiconductor transition point ($\tau_{m\text{-}s}$), PBE bandgap with lattice of 5Å ($\Delta E_{PBE\text{-}5}$), HSE06 bandgap with lattice of 5Å ($\Delta E_{HSE06\text{-}5}$) , spin-polarization and indirect-direct bandgap transition or not for all GSs

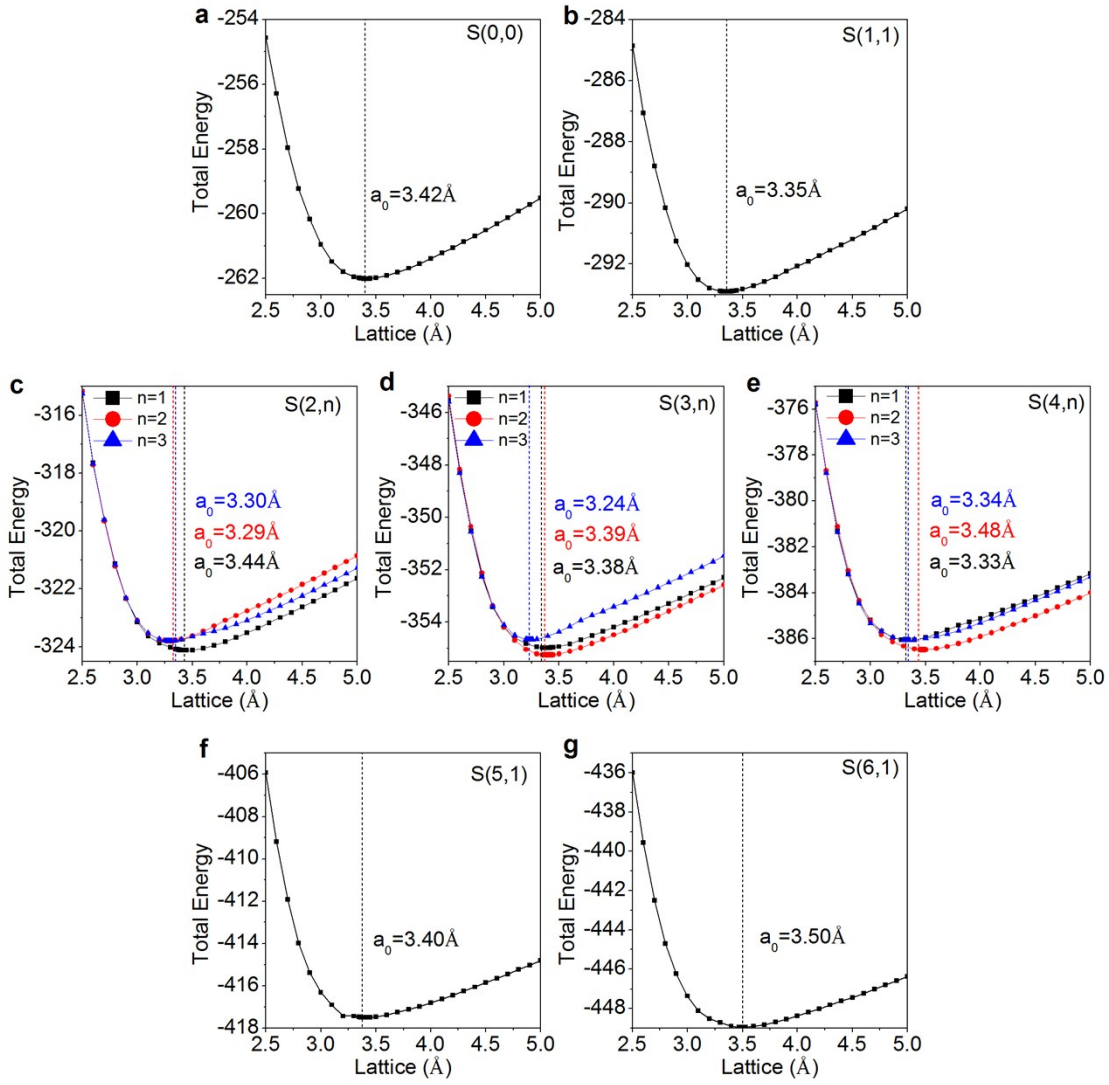

Fig. S1 Total energy as a function of lattices for all GSs.

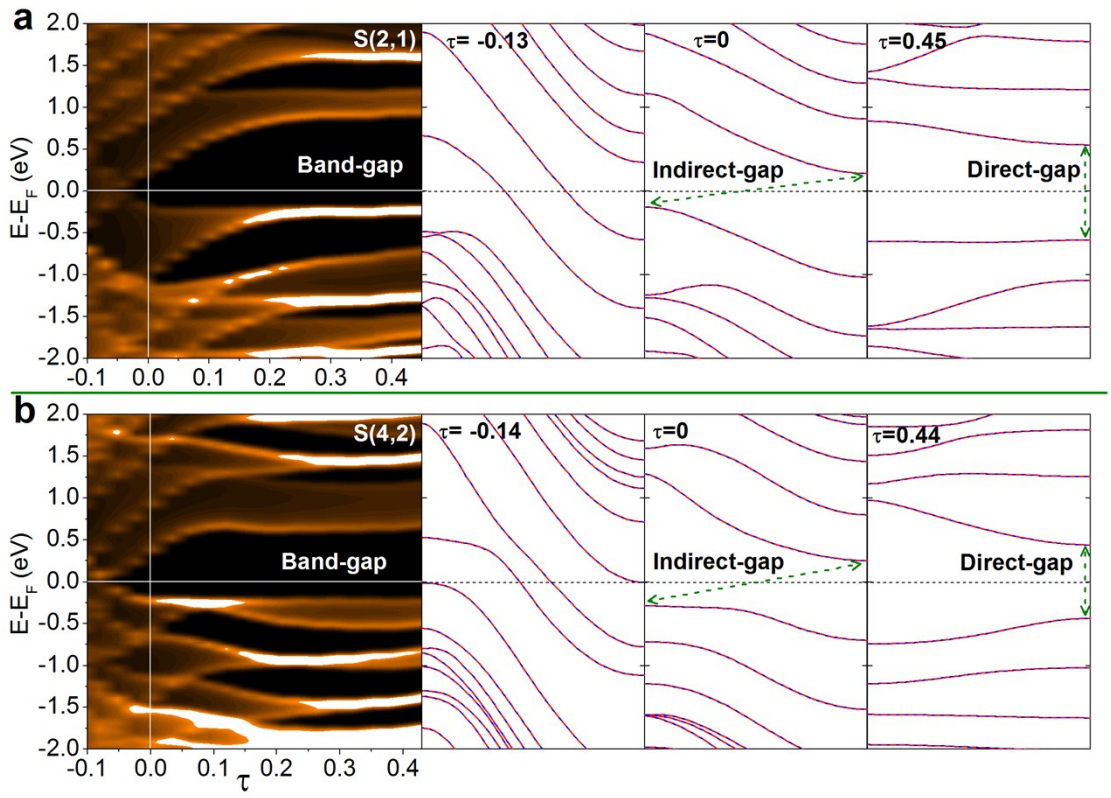

Fig. S2 The evolution of the strain-induced TDOS and BSs for (a) S(2,1) and (b) S(4,2). The orange and black regions in TDOS indicate the intensity variation and energy gap. The black region around Fermi level is bandgap. The VBM and CBM are connected by the dash arrows and Fermi level labeled with dash lines is set to zero for all GSs.

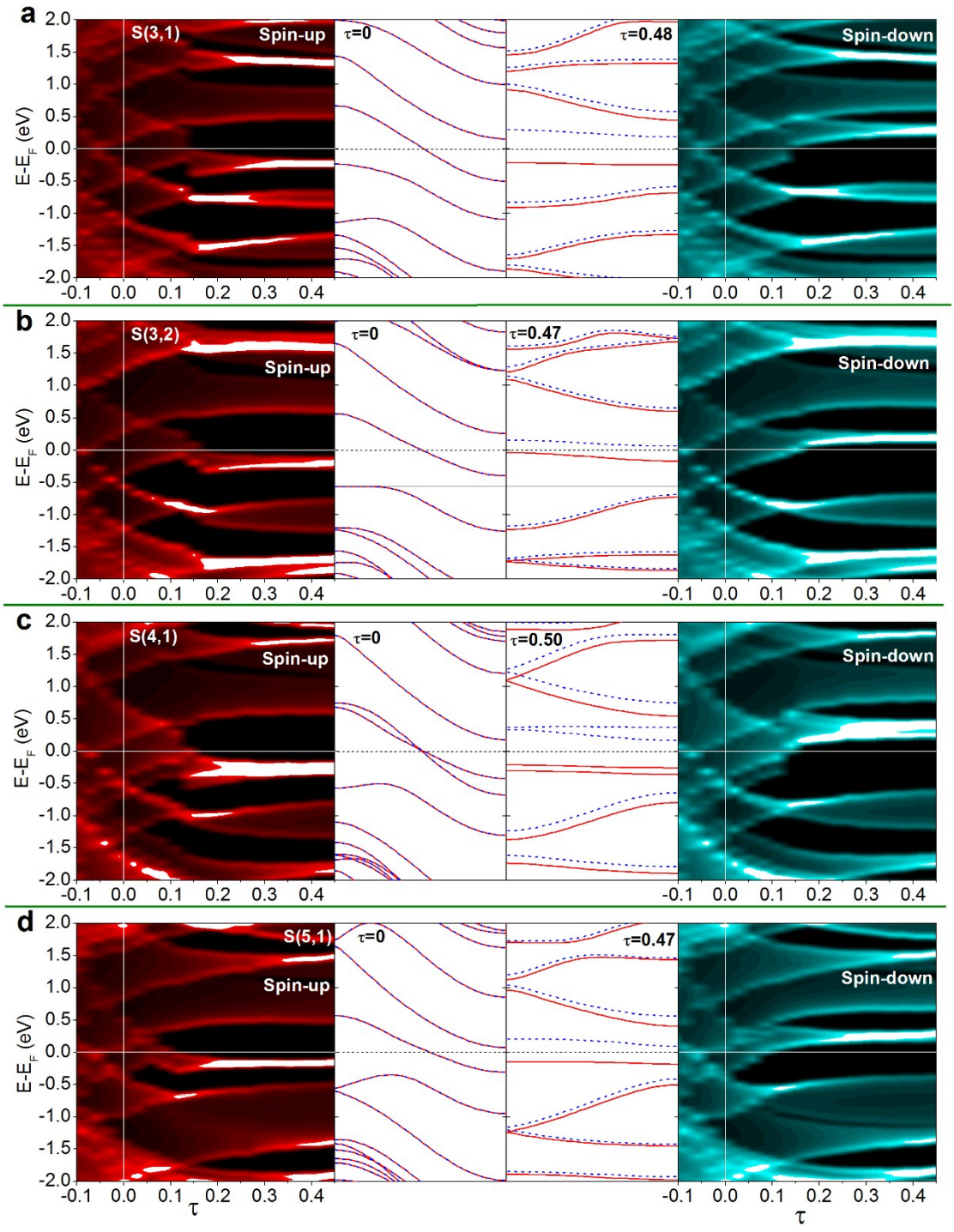

Fig. S3 The evolution of the strain dominated TDOS and BSs of the spin-polarized GSs. (a) S(3,1), (b) S(3,2), (c) S(4,2) and (d) (5,1). The TDOS with red and cyan color represents spin-up and spin-down state respectively. The red and blue lines in BSs represent spin-up bands and spin-down bands, correspondingly.

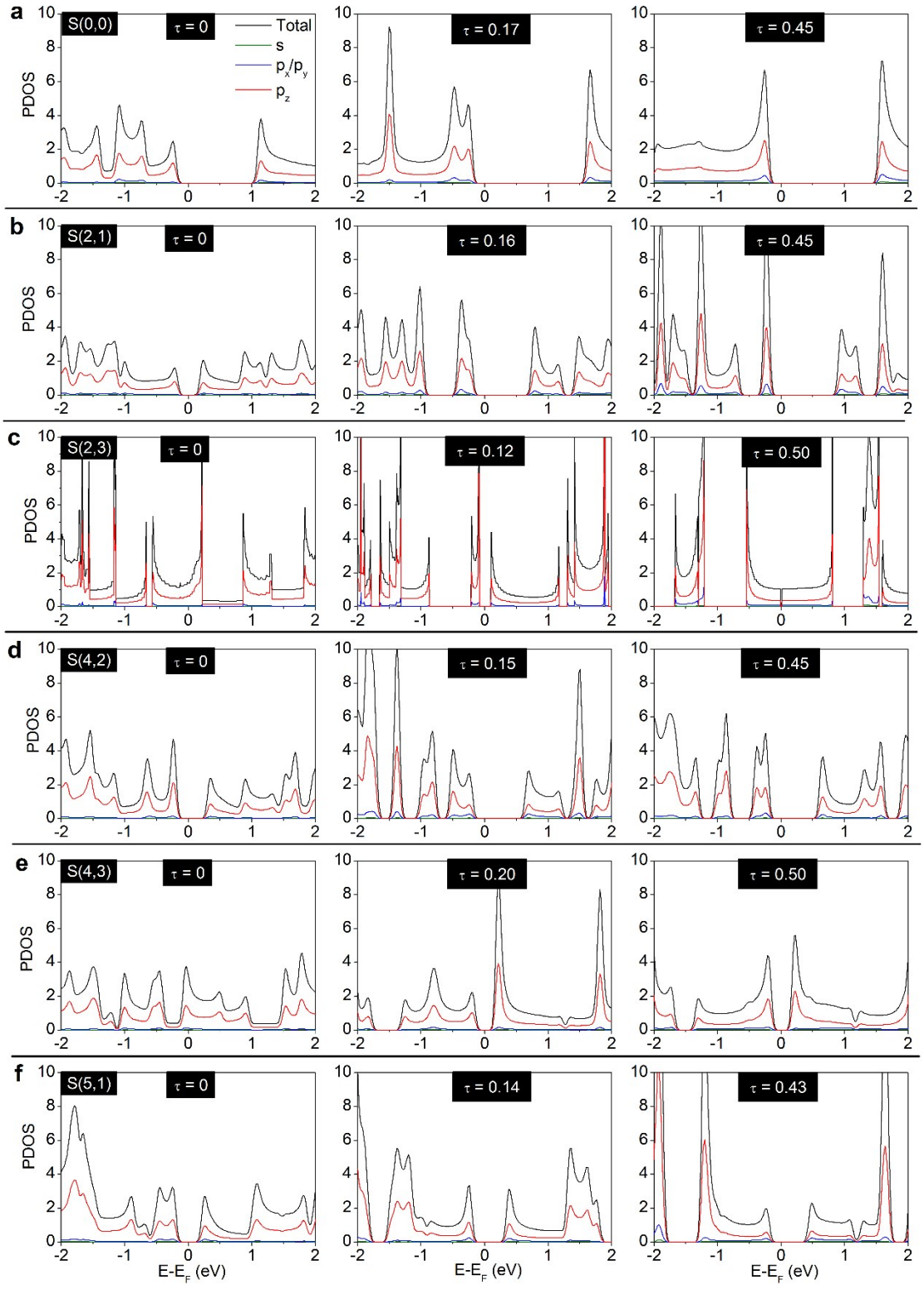

Fig. S4 The variation of the PDOS under selected engineering strain for spin-unpolarized GSs.

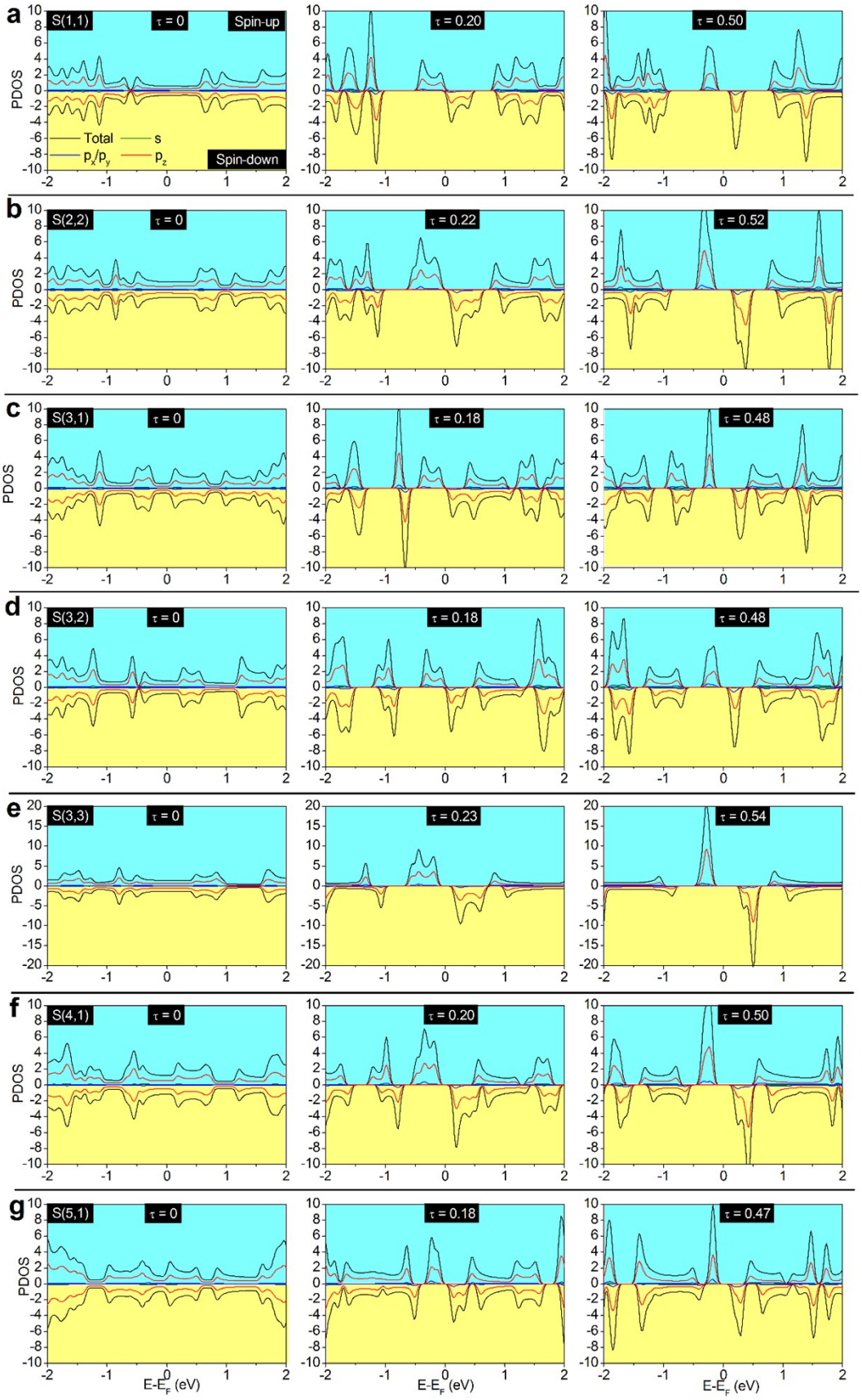

Fig. S5 The variation of the PDOS under selected engineering strain for spin-polarized GSs.

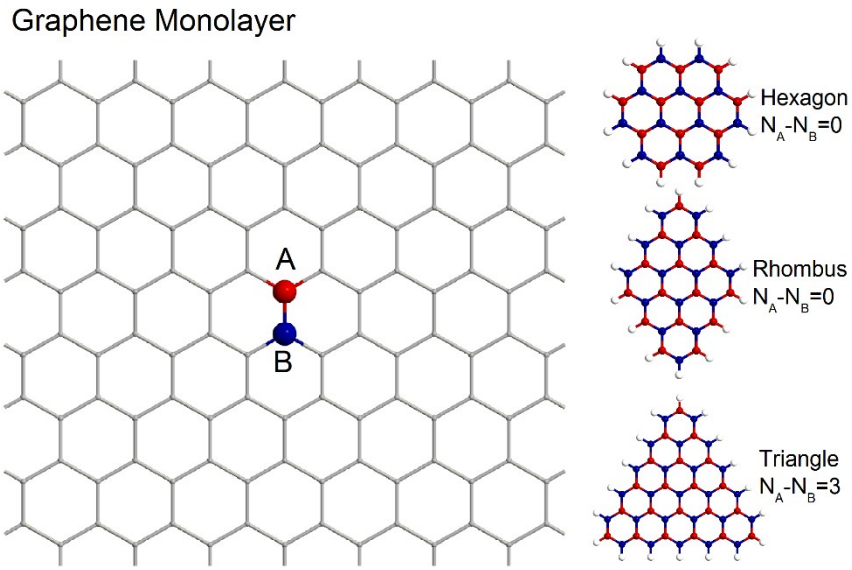

Fig. S6 Schematic representation of graphene with A and B sublattice. The red balls are A sublattices and blue balls are B sublattices. The right panel contains hexagonal, rhombic and triangluar graphene.

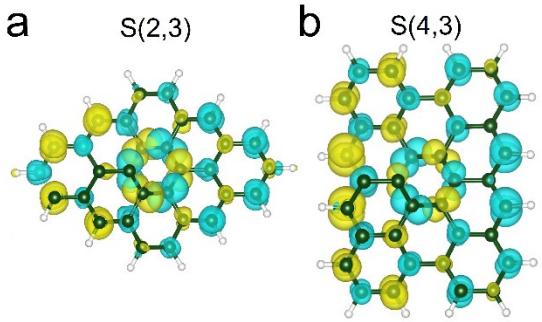

Fig. S7 The spatial distributions of spin-polarized electron density at ground state for S(2,3) and S(4,3). The isosurface value is set to 0.0002Å^{-3}

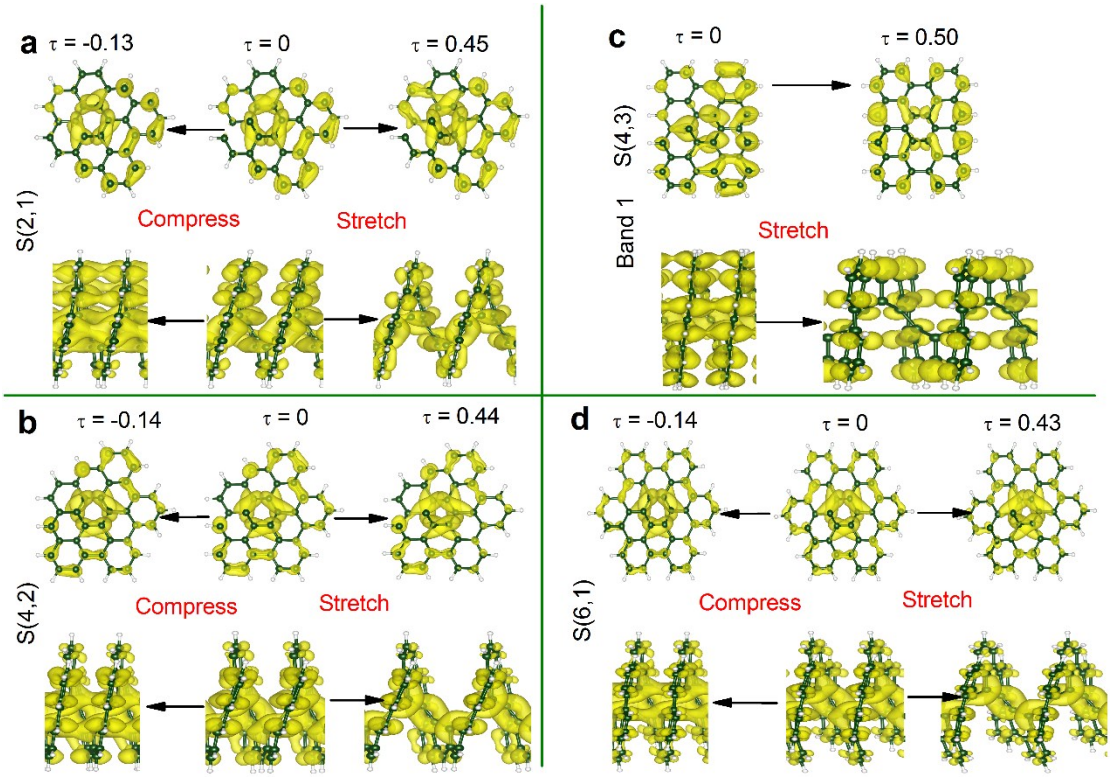

Fig. S8 The topological transformations of the orbital coupling of the subbands near Fermi level for spin-unpolarized GSs under axial strain, equilibrium state and stretch strain. Both of top and side view are contained.

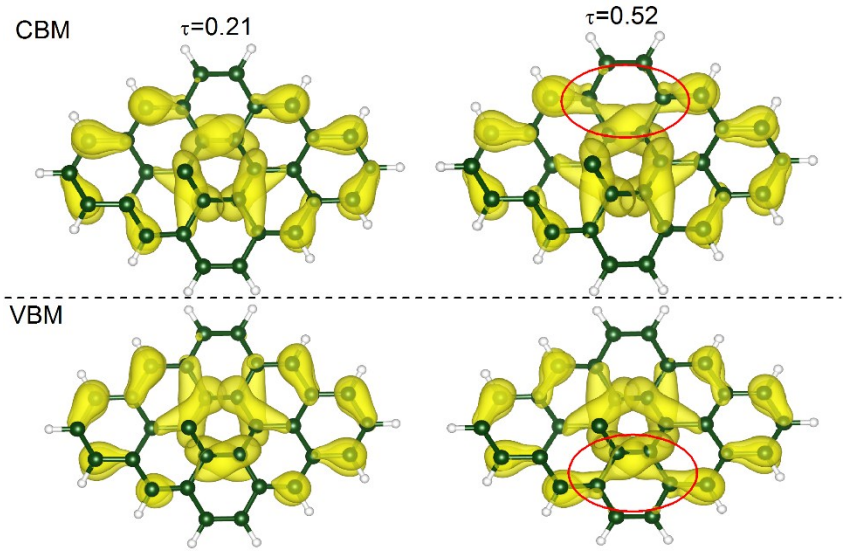

Fig. S9 The localized orbital coupling of CBM and VBM of S(2.3) under τ=0.37 and τ=0.52. The isosurface is set to 0.002 $Å^{-3}$

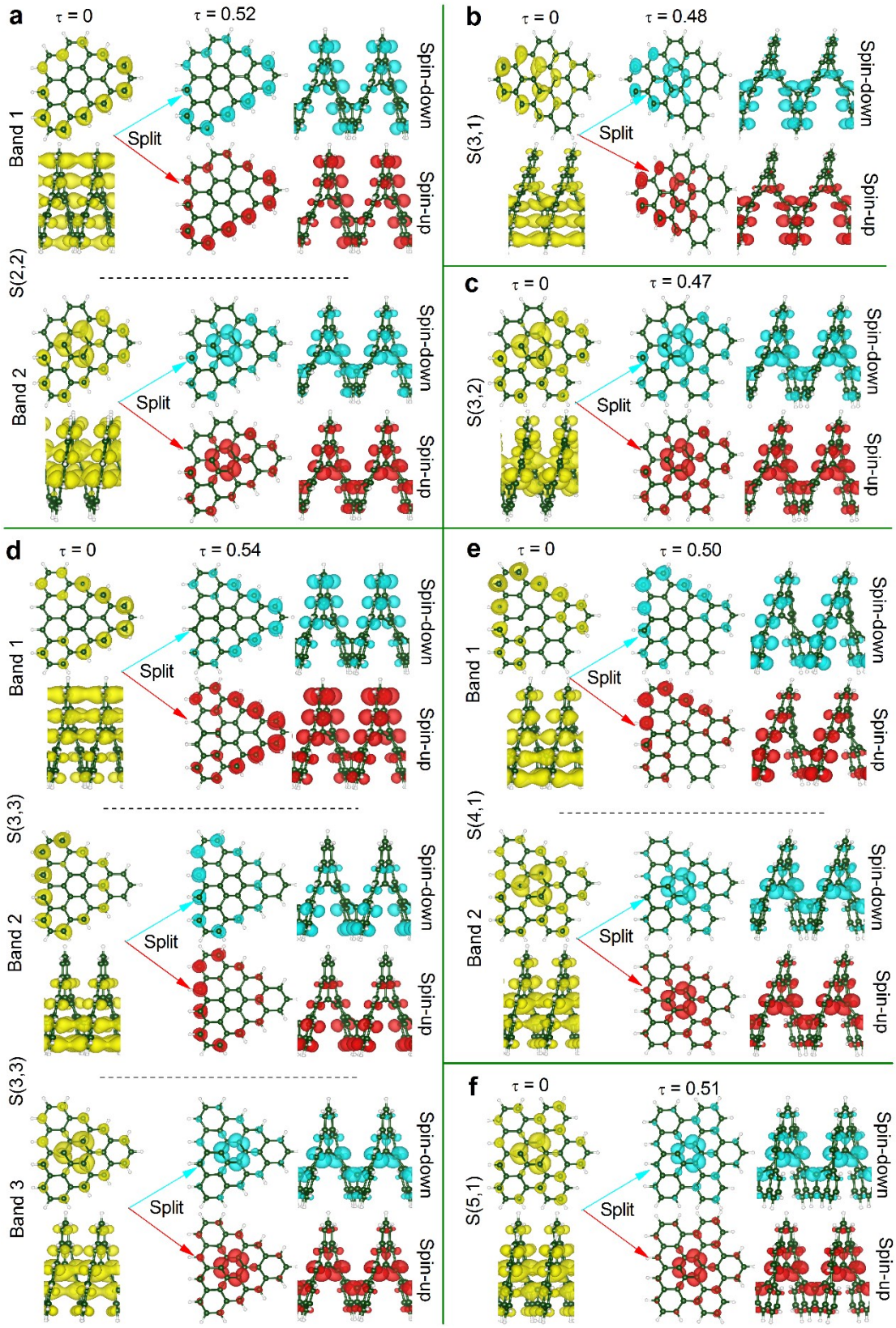

Fig. S10 The topological transformations of the orbital coupling of the subbands near Fermi level for spin-polarized GSs under selected stretch strain

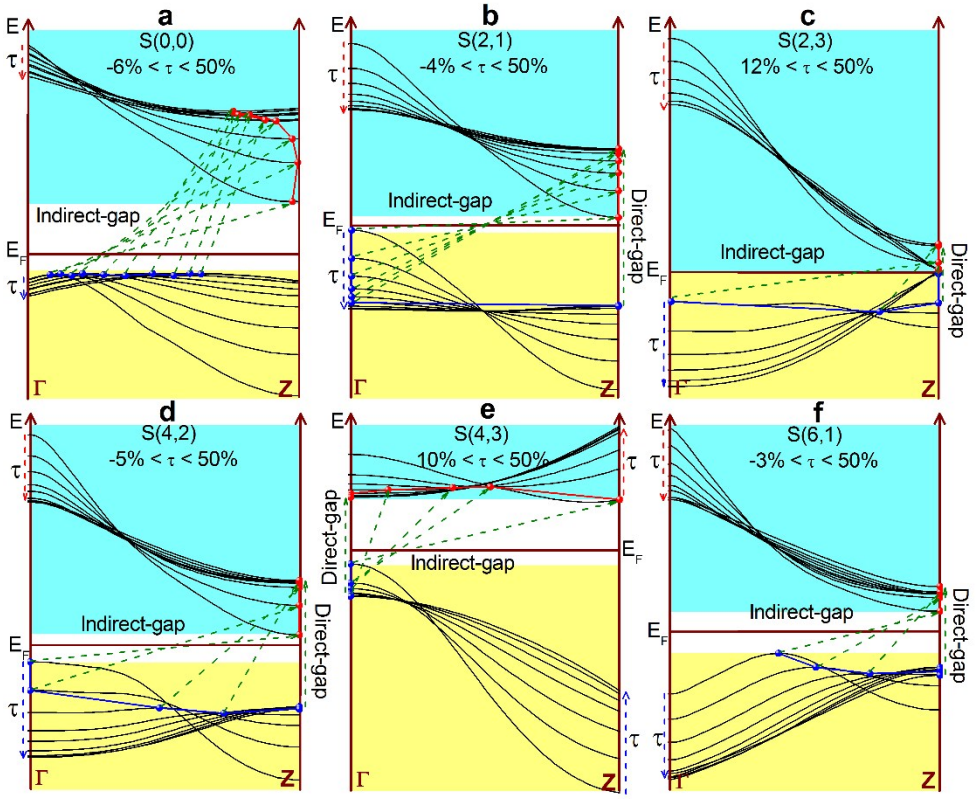

Fig. S11 The variation of the valence band top and conduction band bottom of spin-unpolarized GSs controlled by the axial strain. The blue and red balls indicate the variation of the VBM and CBM repectively. The homologous VBM and CBM at the same strain are connected by the green dash lines. (a) S(0,0); (b) S(2,1); (c) S(2,3); (d) S(4,2); (e) S(4,3); (f) S(6,1). The directions of movements of the bands is labeled by red and blue dash arrows for conduction band and valence band respectively.

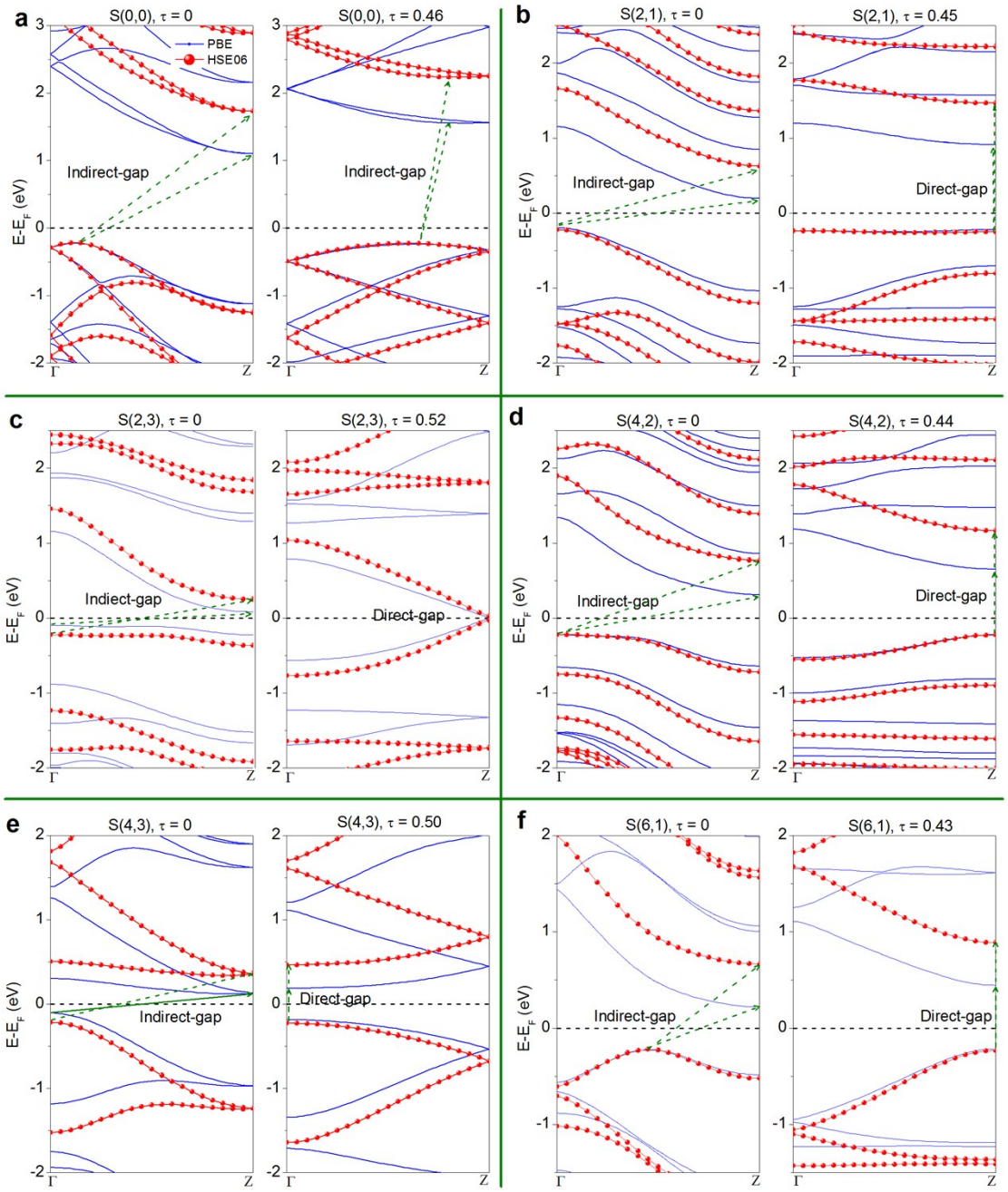

Fig. S12 The comparison of band structures of spin-unpolarized GSs between PBE and HSE06 method.

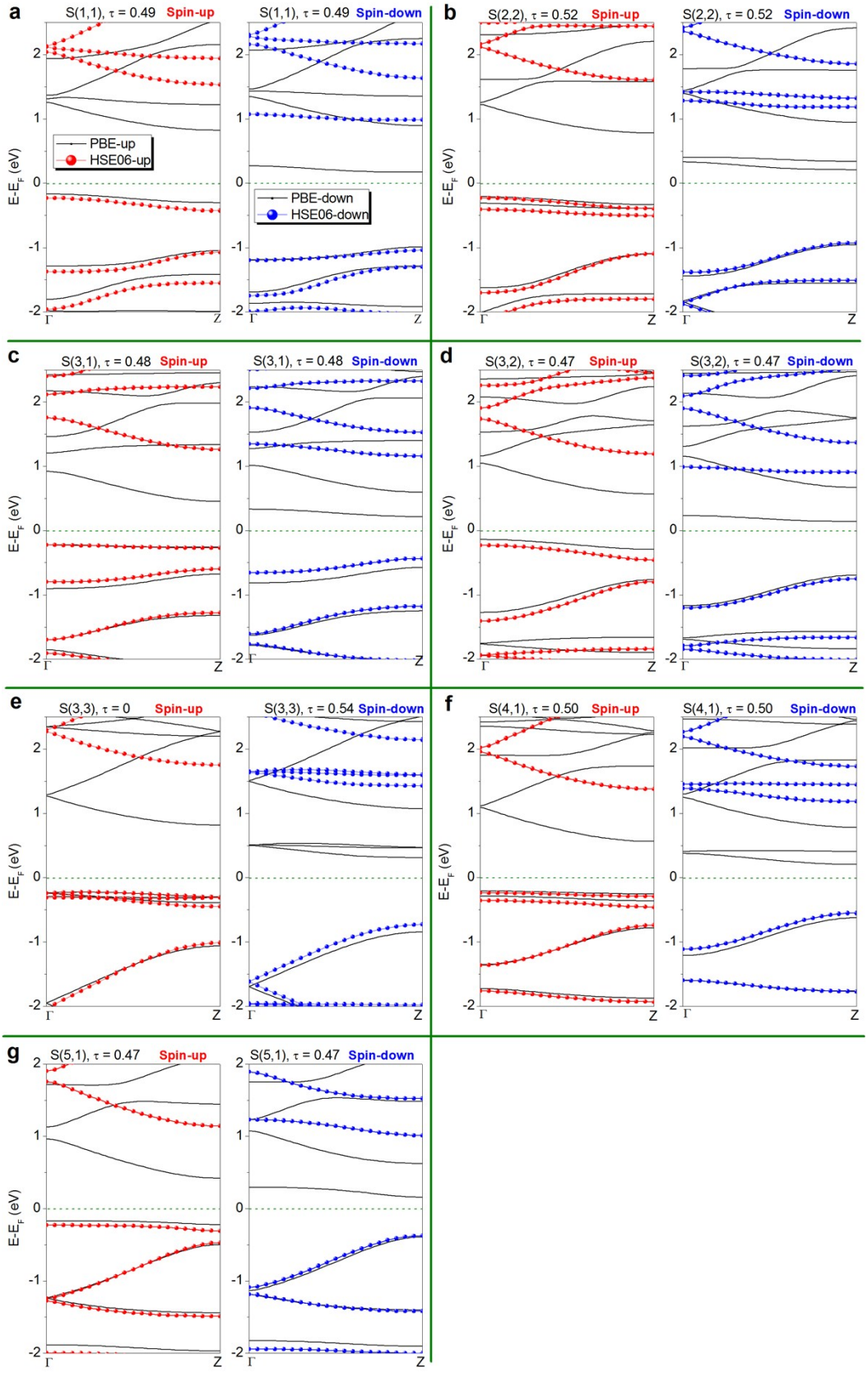

Fig. S13 The comparison of band structures of spin-polarized GSs between PBE and HSE06 method.