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Supplementary Information for:

New Family of Room Temperature Quantum Spin Hall Insulators in Two-Dimensional Germanene films

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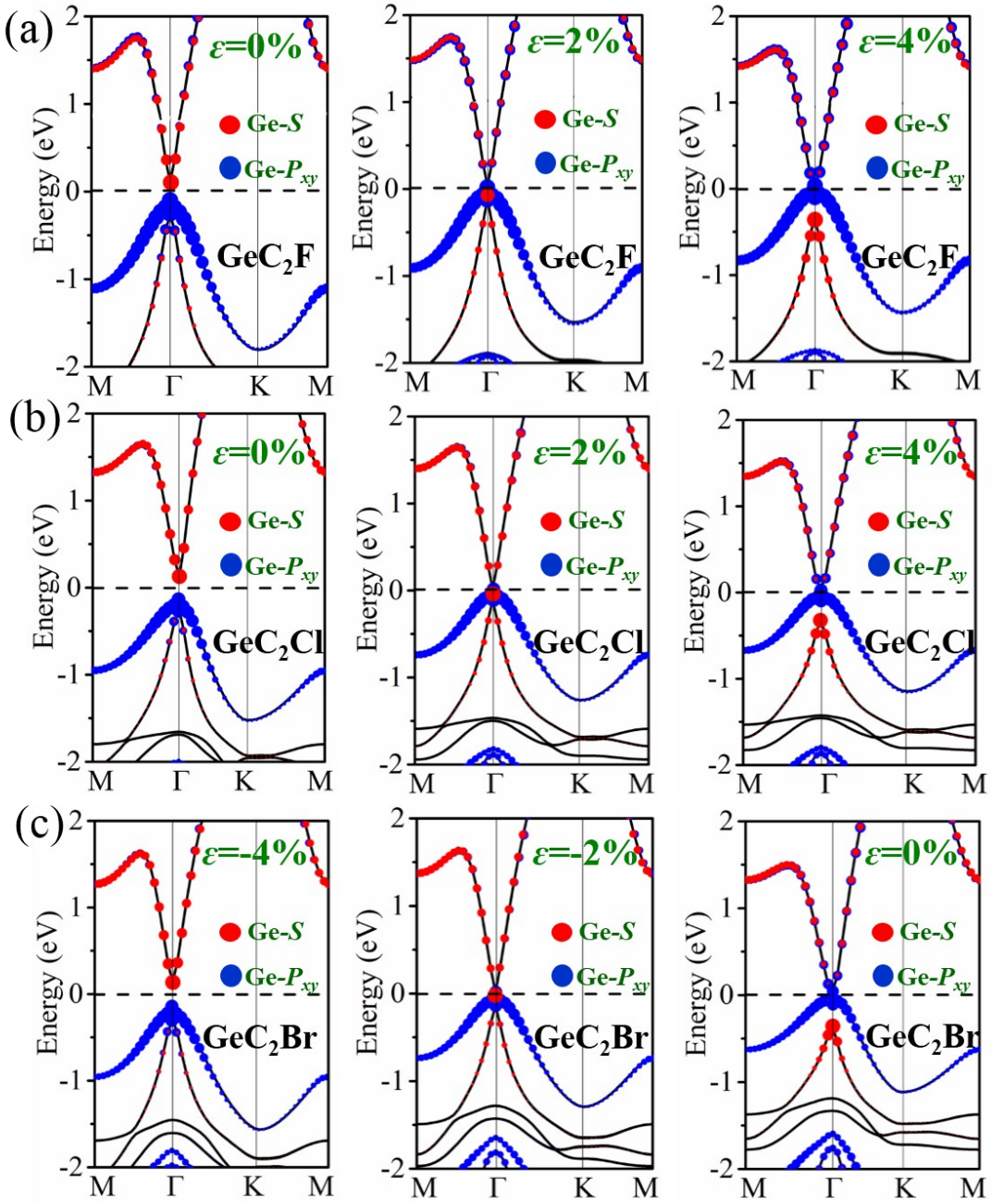

Fig. S1. Orbital-resolved band structures with SOC of (a) GeC_2F and (b) GeC_2Cl under the value of strain ε= 0.0%, 2.0%, 4.0% respectively. (c) GeC_2Br presents orbital-resolved band structures with SOC under the value of strain ε= -4.0%, -2.0%, 0.0% respectively. The red dots represent the contributions from the *s* atomic orbital of Ge atom and the blue dots represent contributions from the p_x and p_y atomic orbitals of Ge atom.

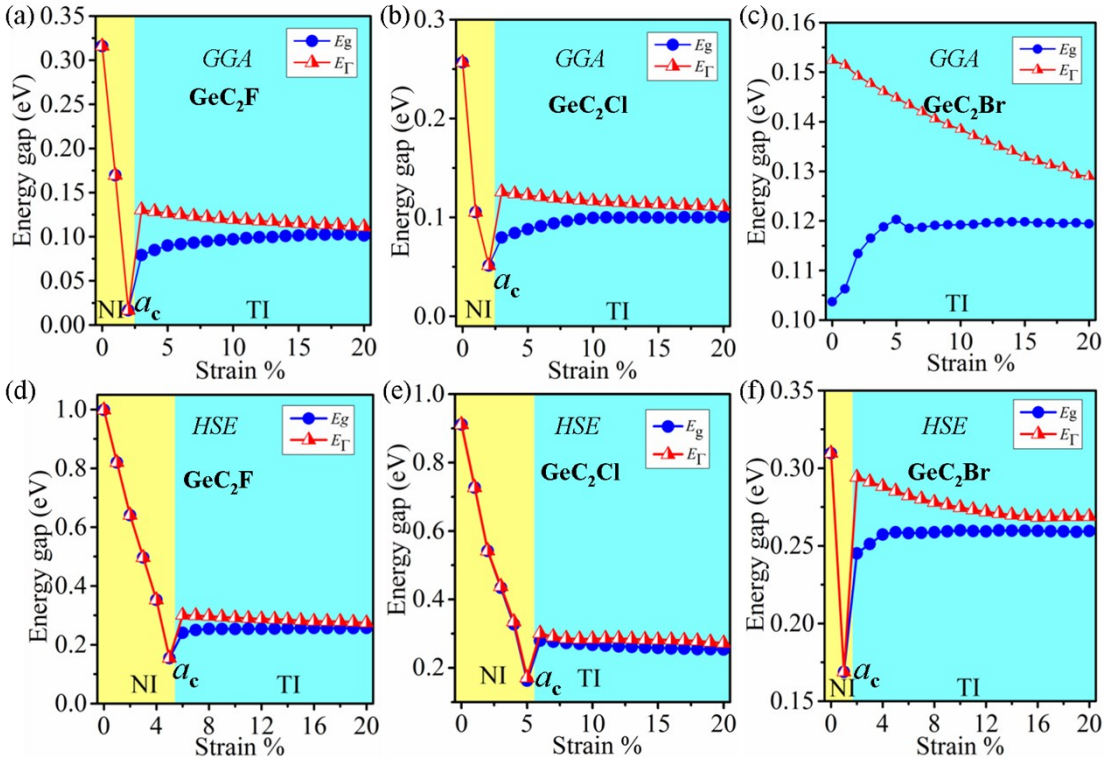

Fig. S2 The calculated energy gaps at Γ point (E_Γ) and the global energy gap (E_g) of GeC_2F (a), GeC_2Cl (b) and GeC_2Br (c) with SOC as a function of external strain by GGA method. The energy gaps at Γ point (E_Γ) and the global energy gap (E_g) of GeC_2F (d), GeC_2Cl (e) and GeC_2Br (f) with SOC as a function of external strain by HSE method. Insets in panel show the trend of band gaps of TI phase as a function of external strain.

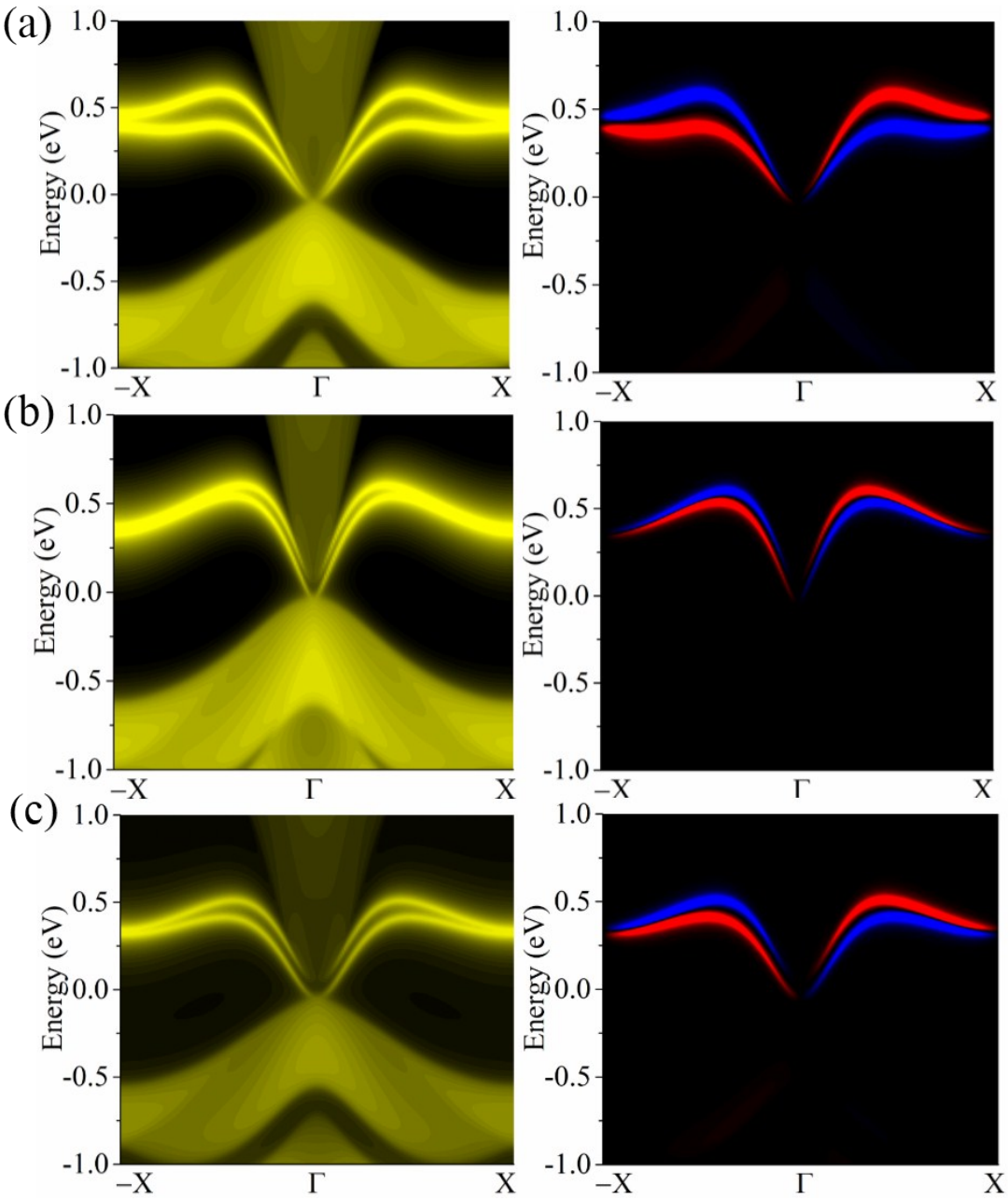

Fig. S3 Total (left panel) and spin (right panel) edge density of states for (a) GeC_2F, (b) GeC_2Cl and (c) GeC_2Br. In the spin edge plot, red/blue lines denote the spin up/down polarization.

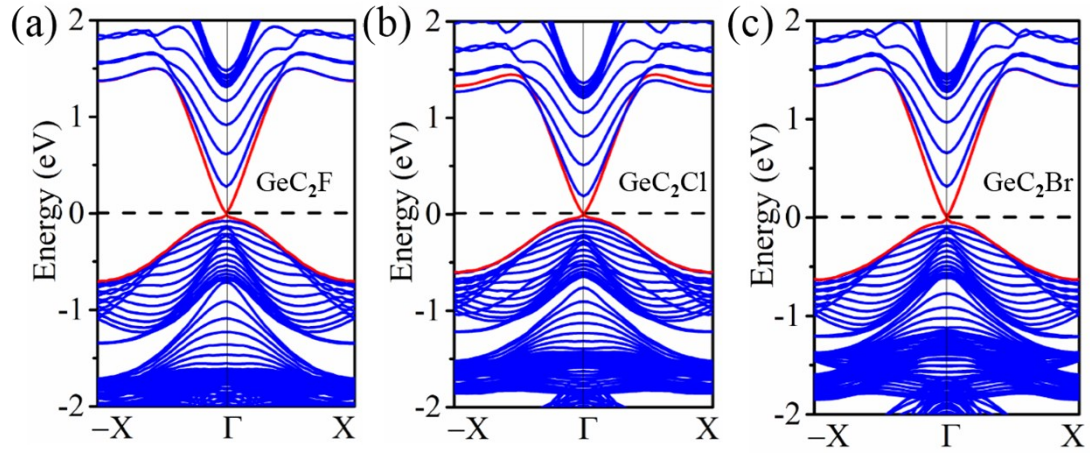

Fig. S4 Calculated electronic band structures of the zigzag-type nanoribbons of (a) GeC_2F (ε = 8.0 %); (b) GeC_2Cl (ε = 8.0 %); and (d) GeC_2Br (ε = 0 %) with SOC.

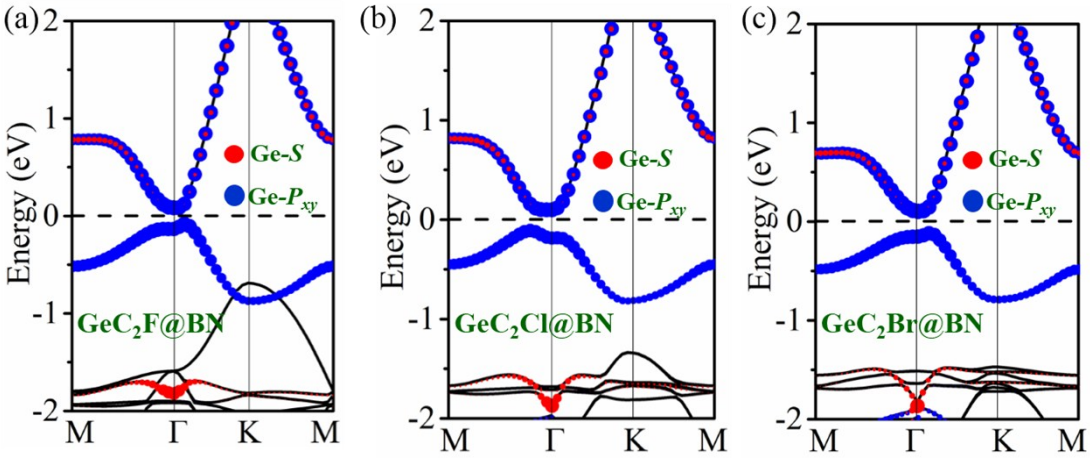

Fig. S5 The orbital-resolved band structures with SOC for (a) GeC_2F@BN, (b) GeC_2Cl@BN and (c) GeC_2I@BN, respectively.