Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

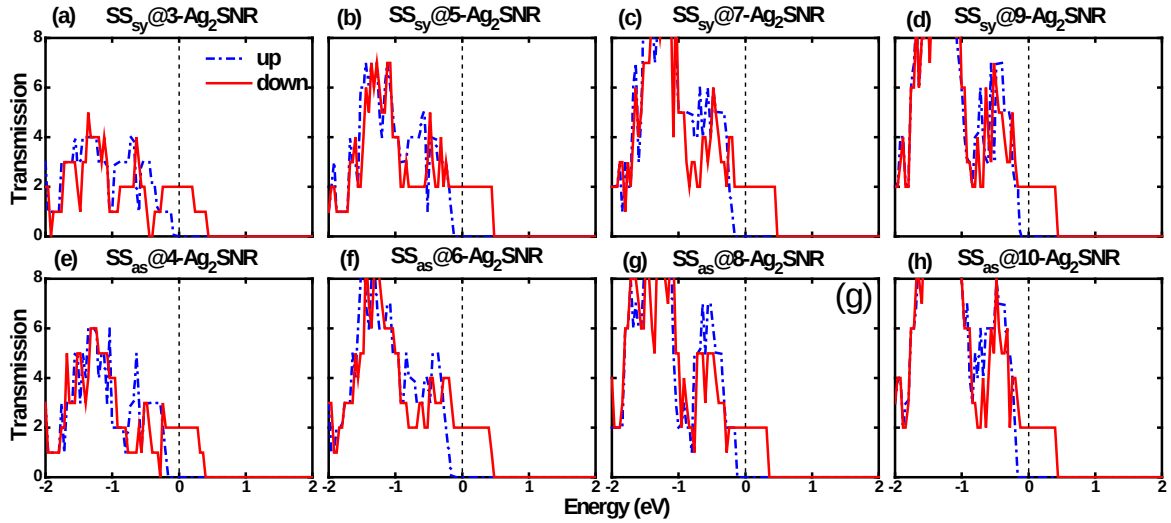

Fig. S1 (a)-(h) Transmissions of SS_{sy}@3-Ag_2SNR, SS_{sy}@5-Ag_2SNR, SS_{sy}@7-Ag_2SNR, SS_{sy}@9-Ag_2SNR, SS_{as}@4-Ag_2SNR, SS_{as}@6-Ag_2SNR, SS_{as}@8-Ag_2SNR and SS_{as}@10-Ag_2SNR, respectively. The blue dashed dot line denotes the spin up transmission, and red solid line denotes spin down one.

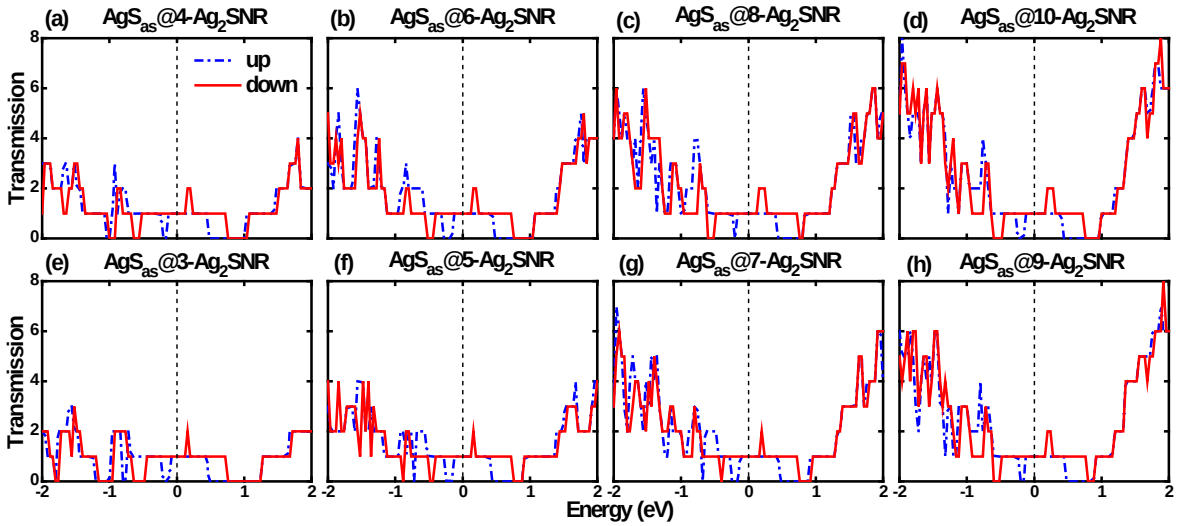

Fig. S2 (a)-(h) Transmissions of AgS_{as}@4-Ag_2SNR, AgS_{as}@6-Ag_2SNR, AgS_{as}@8-Ag_2SNR, AgS_{as}@10-Ag_2SNR, AgS_{sy}@3-Ag_2SNR, AgS_{sy}@5-Ag_2SNR, AgS_{sy}@7-Ag_2SNR and AgS_{sy}@9-Ag_2SNR, respectively. The blue dashed dot line denotes the spin up transmission, and red solid line denotes spin down one.

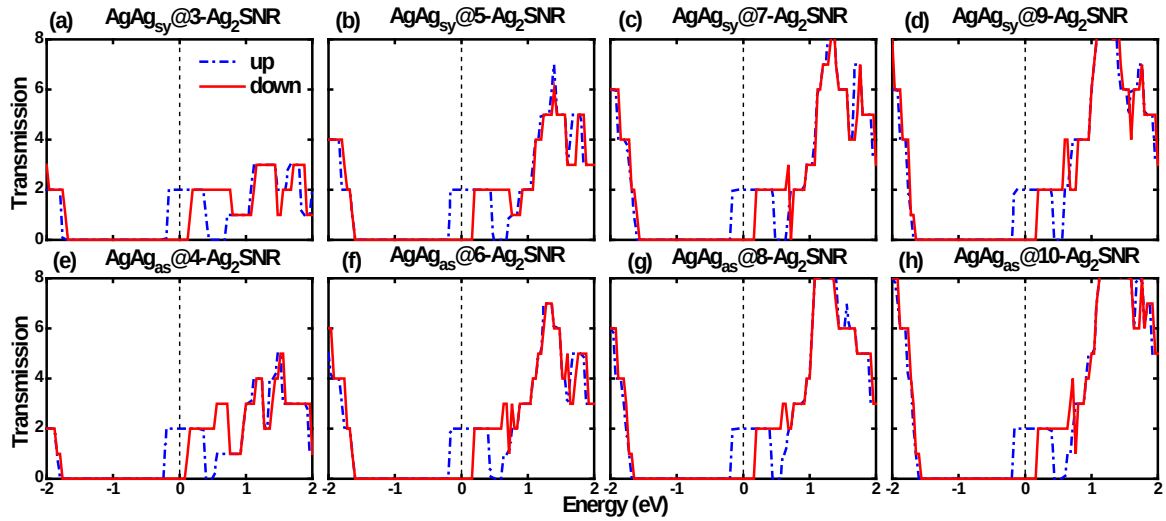

Fig. S3 (a)-(h) Transmissions of AgAg$_{sy}$@3-Ag$_2$SNR, AgAg$_{sy}$@5-Ag$_2$SNR, AgAg$_{sy}$@7-Ag$_2$SNR, AgAg$_{sy}$@9-Ag$_2$SNR, AgAg$_{as}$@4-Ag$_2$SNR, AgAg$_{as}$@6-Ag$_2$SNR, AgAg$_{as}$@8-Ag$_2$SNR and AgAg$_{as}$@10-Ag$_2$SNR, respectively. The blue dashed dot line denotes the spin up transmission, and red solid line denotes spin down one.

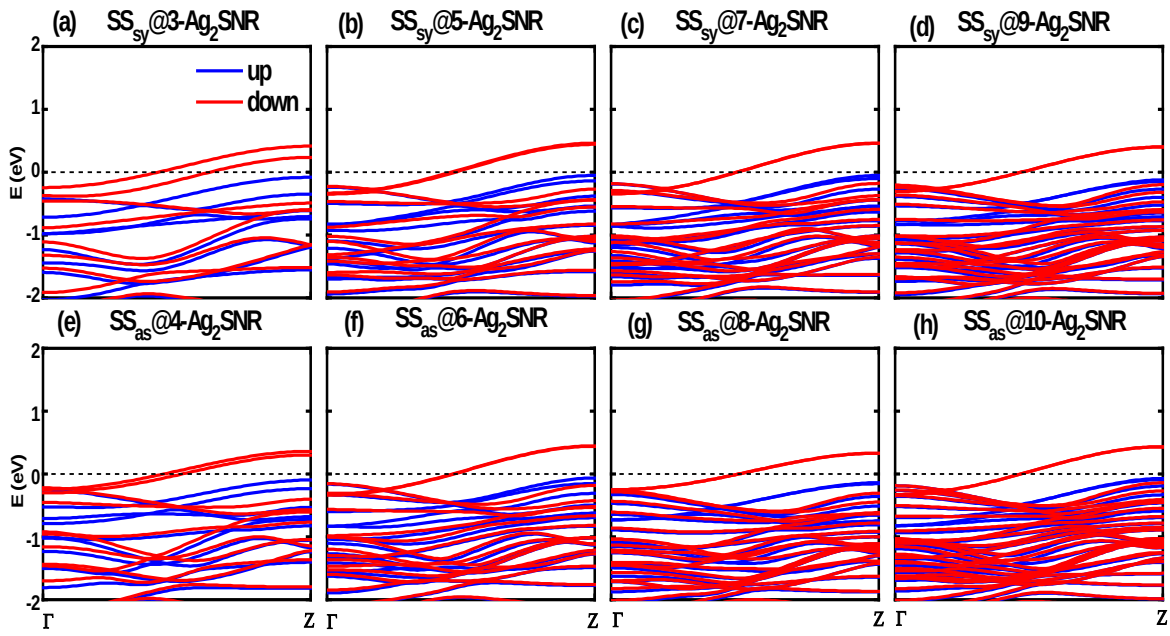

Fig. S4 (a)-(h) Band structures of SS$_{sy}$@3-Ag$_2$SNR, SS$_{sy}$@5-Ag$_2$SNR, SS$_{sy}$@7-Ag$_2$SNR, SS$_{sy}$@9-Ag$_2$SNR, SS$_{as}$@4-Ag$_2$SNR, SS$_{as}$@6-Ag$_2$SNR, SS$_{as}$@8-Ag$_2$SNR and SS$_{as}$@10-Ag$_2$SNR, respectively. The blue solid line denotes the spin up bands, and red solid line denotes spin down one.

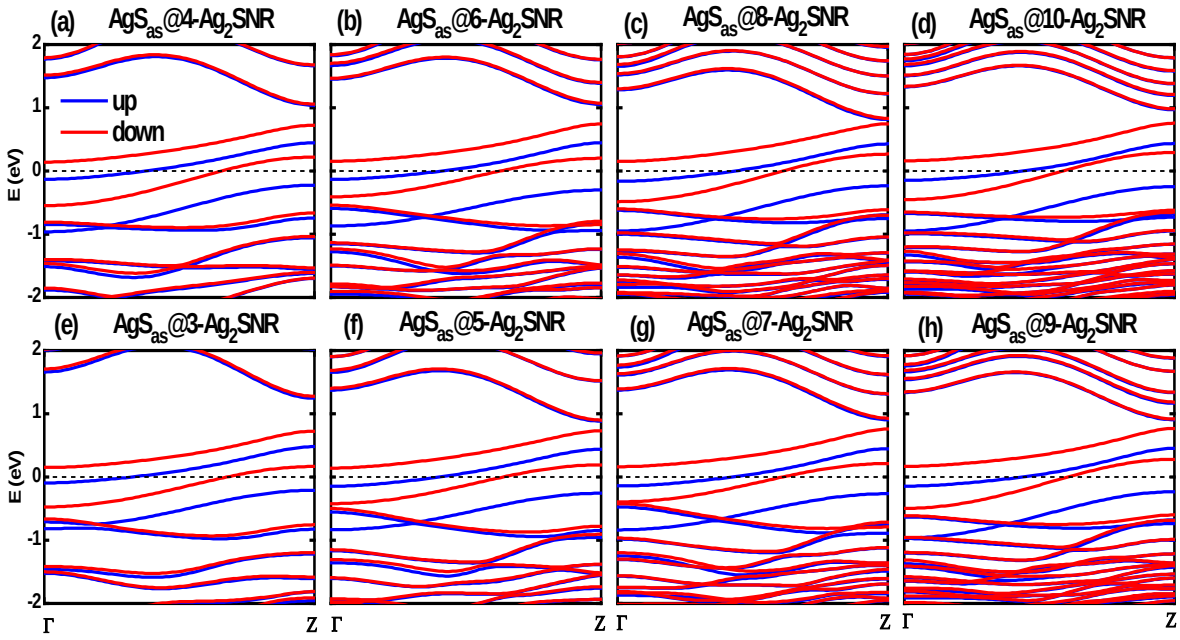

Fig. S5 (a)-(h) Band structures of AgS_{as}@4-Ag_2SNR, AgS_{as}@6-Ag_2SNR, AgS_{as}@8-Ag_2SNR, AgS_{as}@10-Ag_2SNR, AgS_{sy}@3-Ag_2SNR, AgS_{sy}@5-Ag_2SNR, AgS_{sy}@7-Ag_2SNR and AgS_{sy}@9-Ag_2SNR, respectively. The blue solid line denotes the spin up bands, and red solid line denotes spin down one.

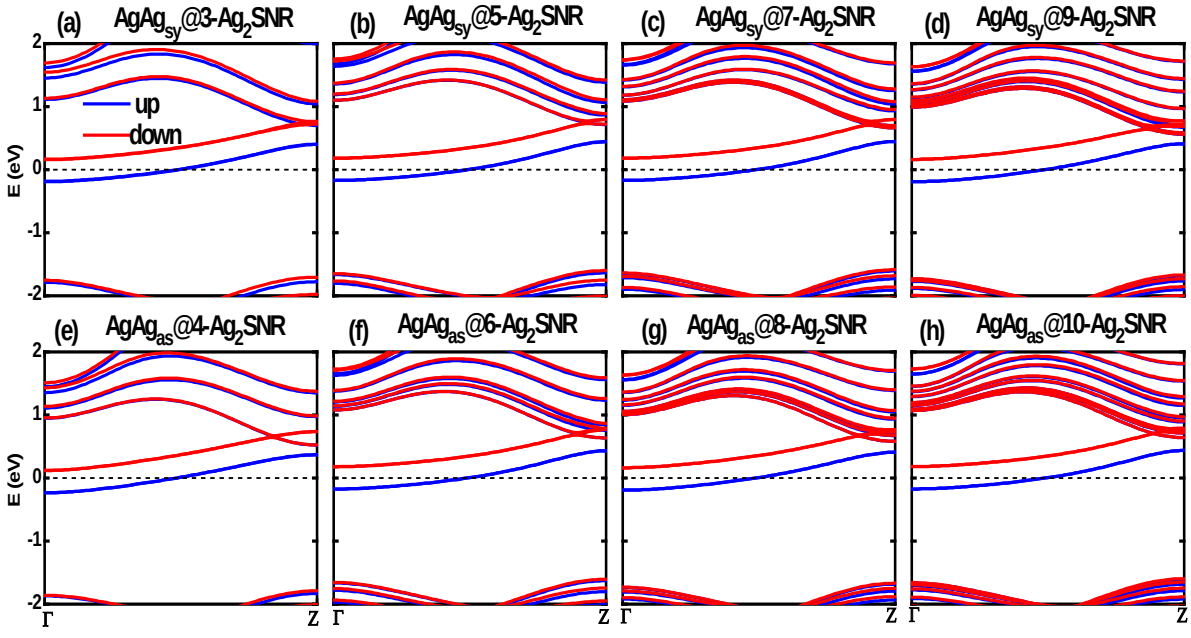

Fig. S6 (a)-(h) Band structures of $AgAg_{sy}$@3-Ag_2SNR, $AgAg_{sy}$@5-Ag_2SNR, $AgAg_{sy}$@7-Ag_2SNR, $AgAg_{sy}$@9-Ag_2SNR, $AgAg_{as}$@4-Ag_2SNR, $AgAg_{as}$@6-Ag_2SNR, $AgAg_{as}$@8-Ag_2SNR and $AgAg_{as}$@10-Ag_2SNR, respectively. The blue solid line denotes the spin up bands, and red solid line denotes spin down one.

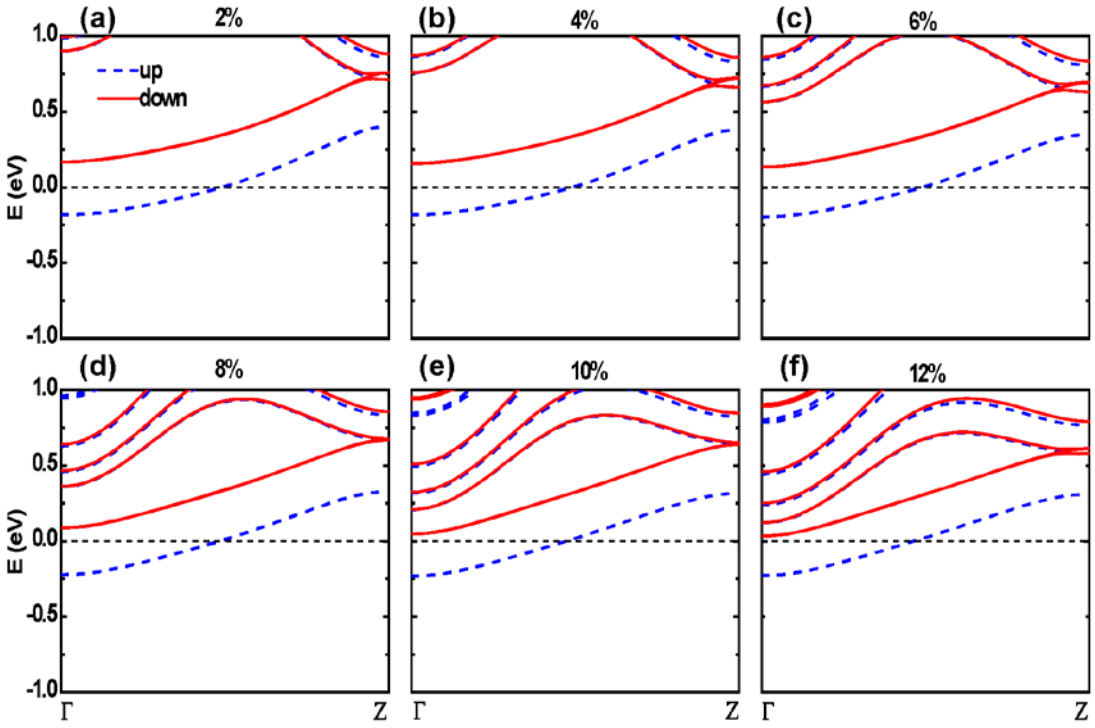

Fig. S7 (a)-(f) The band structures of $AgAg_{sy}$@5-Ag_2SNR under the applied tensile strains (from 2% to 12%). The blue dashed line denotes the spin up band structure, and the red solid line denotes the spin down one. The Fermi level (E_F) is set to 0.

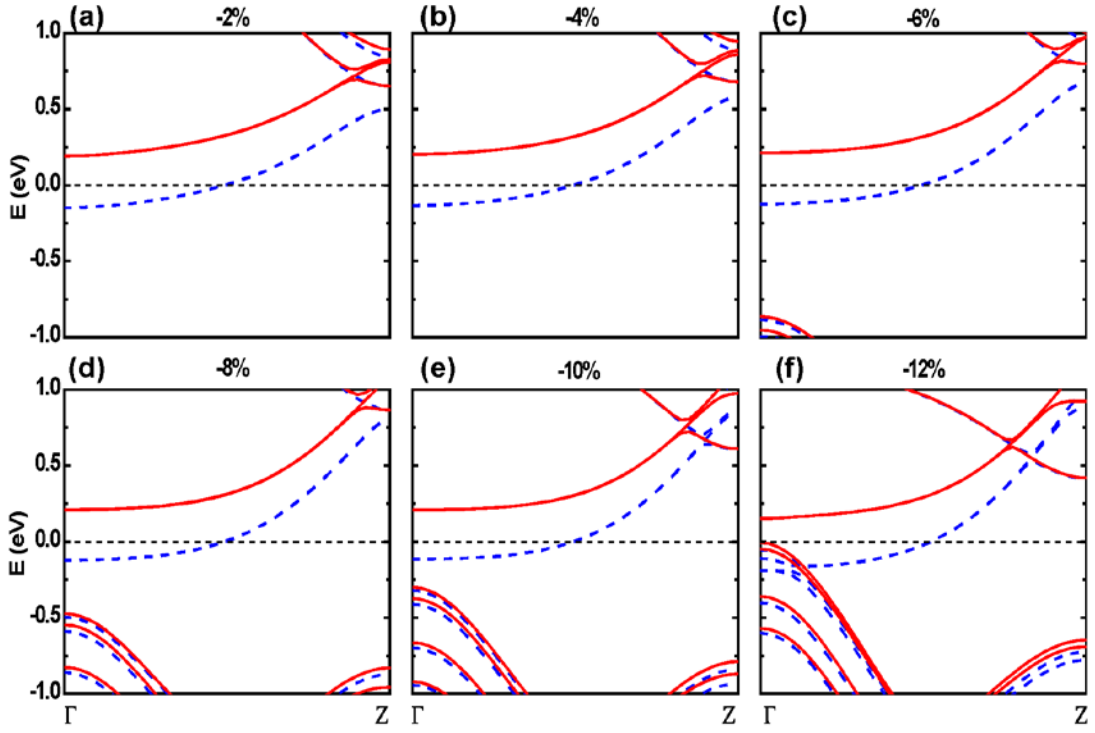

Fig. S8 (a)-(f) The band structures of $AgAg_{sy}$@5-Ag_2SNR under the applied compressible strains (from -2% to -12%). The blue dashed line denotes the spin up band structure, and the red solid line denotes the spin down one. The Fermi level (E_F) is set to 0.

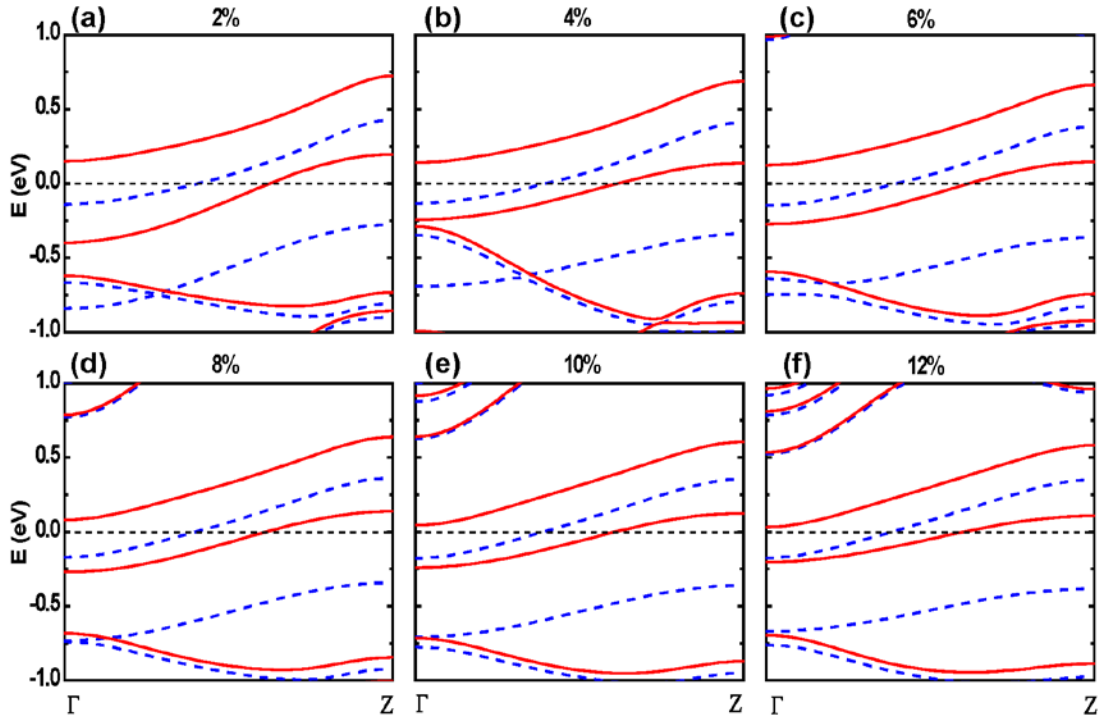

Fig. S9 (a)-(f) The band structures of AgS_{as}@6-Ag_2SNR under the applied tensile strains (from 2% to 12%). The blue dashed line denotes the spin up band structure, and the red solid line denotes the spin down one. The Fermi level (E_F) is set to 0.

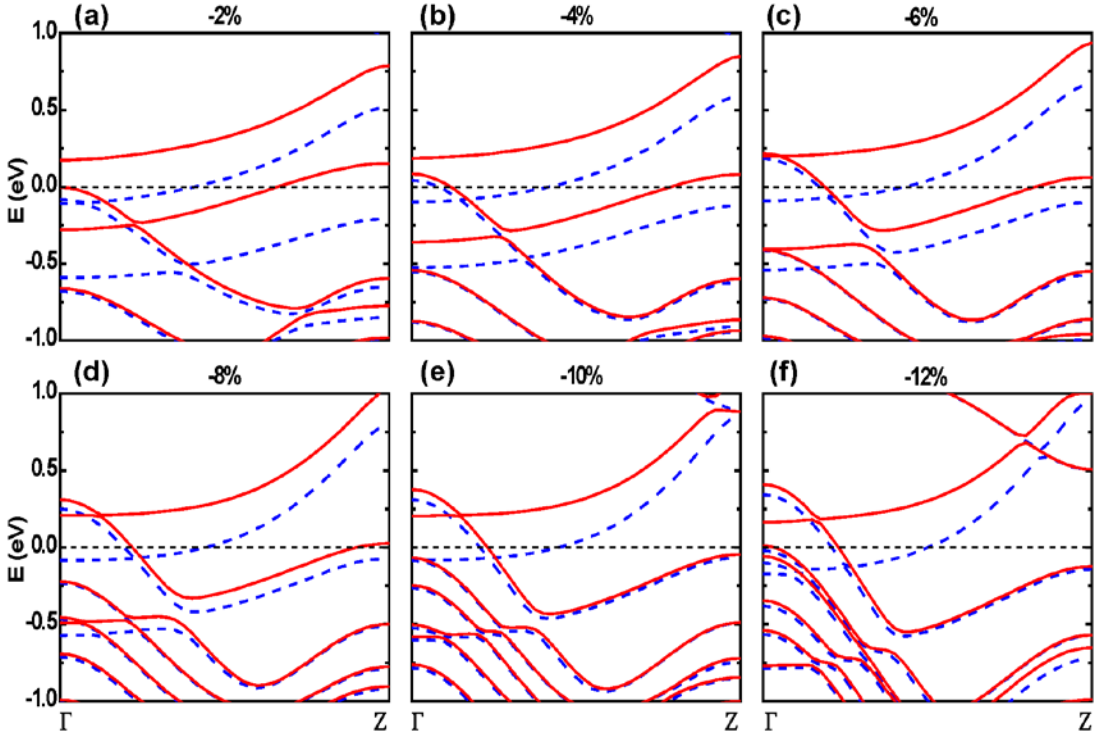

Fig. S10 (a)-(f) The band structures of AgS_{as}@6-Ag_2SNR under the applied compressible strains (from -2% to -12%). The blue dashed line denotes the spin up band structure, and the red solid line denotes the spin down one. The Fermi level (E_F) is set to 0.

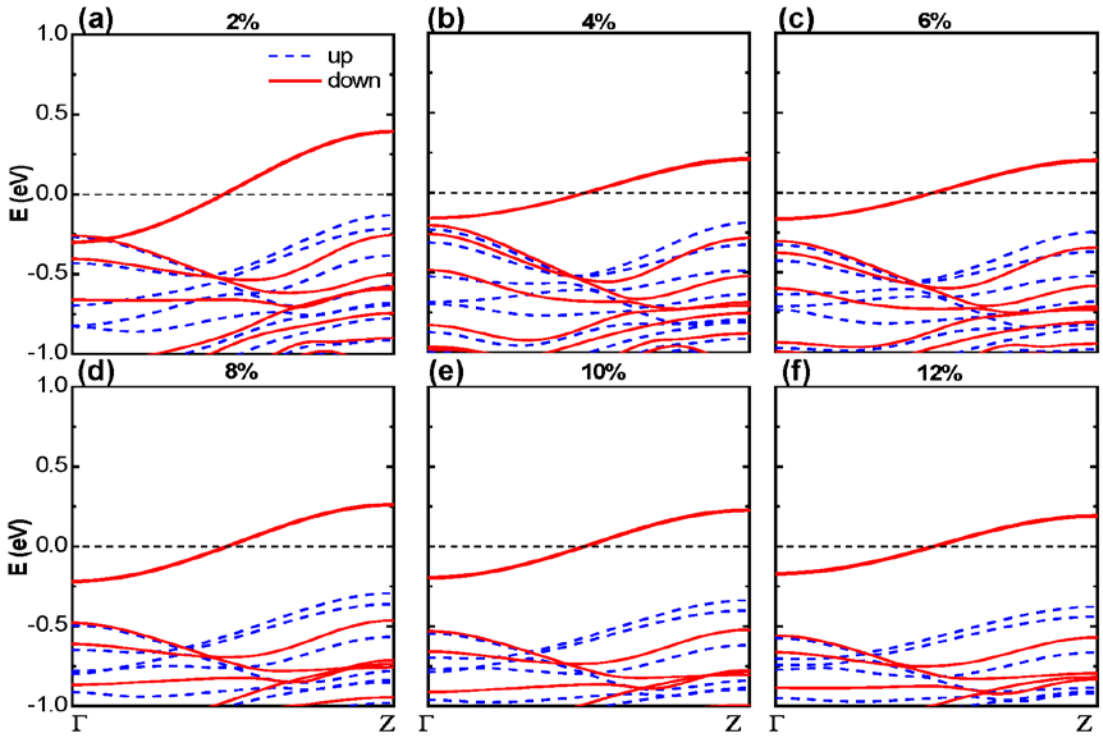

Fig. S11 (a)-(f) The band structures of SS_{as}@6-Ag_2SNR under the applied tensile strains (from 2% to 12%). The blue dashed line denotes the spin up band structure, and the red solid line denotes the spin down one. The Fermi level (E_F) is set to 0.

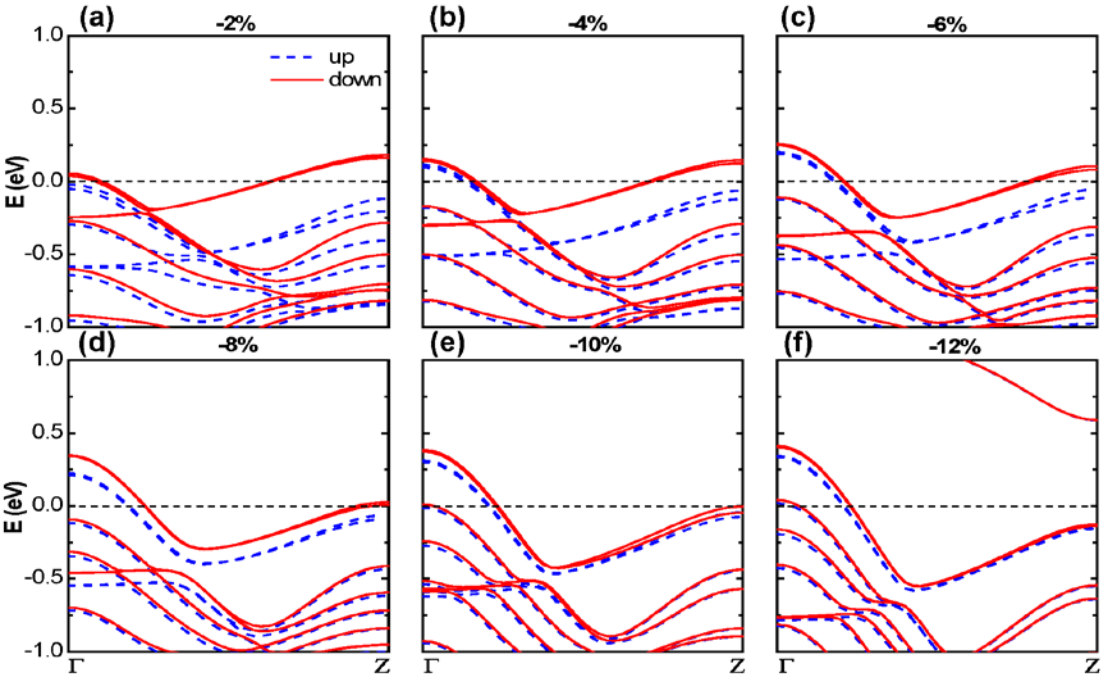

Fig. S12 (a)-(f) The band structures of SS_{as}@6-Ag_2SNR under the applied compressible strains (from -2% to -12%). The blue dashed line denotes the spin up band structure, and the red solid line denotes the spin down one. The Fermi level (E_F) is set to 0.