Electronic supplementary information (ESI) available:

Stress Induced Half-Metallicity in Surface Defected Germanium Nanowire

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Validation of our method:

The underestimation of band gap is a well known phenomenon with DFT GGA. Heyd et al. (*J. Chem. Phys.* **2005**, *123*, 174101) showed that the DFT GGA methods underestimate the small-band gap systems like bulk Ge and predicted to be quasi-metallic. To verify that the conclusions drawn from our calculations are not affected by the underestimation of the band gap of bulk Ge in standard DFT GGA calculations, we have performed GGA+U calculations (S. L. Dudarev et al., *Phys. Rev. B* **1998**, *57*, 1505) for bulk Ge and surface defected GeNW **2c**. For bulk Ge, we obtained the best value of the U-J parameter is 8.0. The calculated band gap of bulk Ge is 0.40 eV with the value of 8.0 for the U-J parameter. The calculated band gap of bulk Ge is close to the experimental value of ~0.66 eV. We apply the U-J parameter of 8.0 obtained from bulk Ge calculation to calculate the surface defected GeNW **2c**. The calculated results predict the half-metallic nature for the surface defected GeNW **2c** with net magnetic moment of 2.00 μ_B, similarly to the standard DFT GGA calculations. The results of which are shown below in Figs 1 and 2. The different energy gaps of GeNW **2c** calculated using the two methods are shown in Fig. 2 for comparison. The results show that both the methods predict the half-metallic GeNW. This suggest that though the DFT GGA method underestimates the band gap of bulk Ge, GGA method can be used to predict the nature of GeNWs.

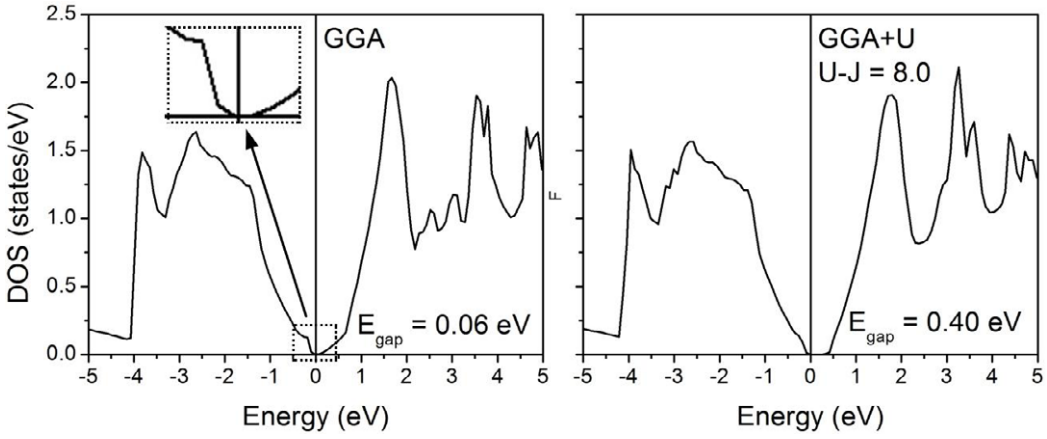

Figure 1. Density-of-state of bulk Ge calculated using DFT GGA and GGA+U methods.

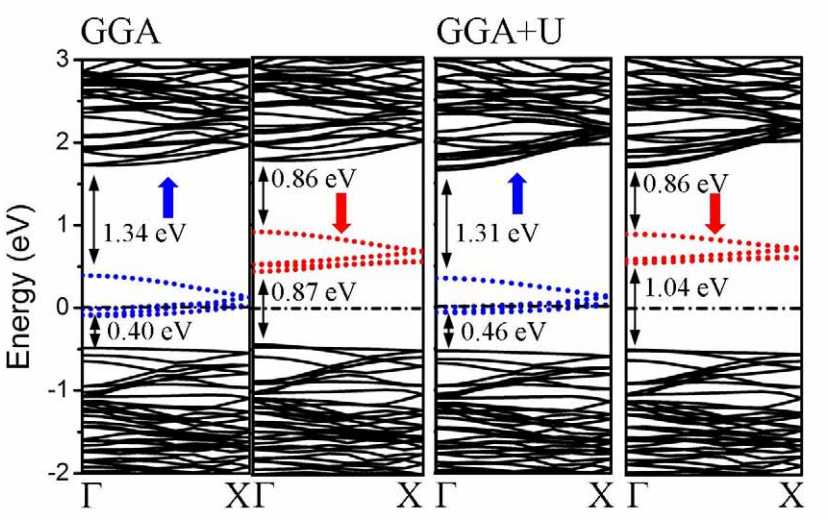

Figure 2. Band structures of surface defected GeNW **2c** with net magnetic moment of 2.00 μ_B calculated using GGA and GGA+U methods.

Table S1 The calculated defect generation energies of SDB defects [a] per SDB (E_{Gen}^{SDB}), and formation energy (E_{form}), net magnetic moments (in μ_B) per unit cell and band gap (E_{gap}) of surface defected GeNWs

GeNW	E_{Gen}^{SDB} per SDB (eV)	E_{form} (eV/Ge atoms)	Net magnetic moment (μ_B)	E_{gap}	
				Spin-up	Spin-down
2h	0.72	0.23	1.96	1.47	0.81
2i	0.62	0.23	0.00	0.29	0.29
2j	0.70	0.23	0.00	0.13	0.13
2k	0.92	0.24	2.00	1.60	0.85
2l	0.92	0.24	2.00	1.58	0.91
2m	0.92	0.24	2.00	1.54	0.88
2n	0.76	0.23	0.00	0.68	0.68
2o	-0.04	0.18	0.00	2.01	
2p	0.91	0.24	2.00	1.64	0.91
2q	0.90	0.24	2.00	1.70	0.97
2r	0.91	0.24	2.00	1.60	0.88
4c	0.91	0.30	0.00	0.11	0.11
4d	0.92	0.30	3.95	1.64	0.68
4e	0.79	0.28	0.00	0.59	0.59
8a	0.56	0.33	0.00	0.00	0.00
8b	0.40	0.29	0.00	0.42	0.42

Table S2 The total energies of optimized surface defected GeNWs and their magnetic states

GeNW	Total Energies (eV)[a]	States[b]
1a	-429.654281	FM [-429.654344] [c]
1b	-429.259966	FM [-429.260053]
1c	-429.284768	FM [-429.284742]
2a	-421.448723	wFM [-421.448702]
2b	-423.205380	AFM [-423.205351]
2c	-421.437060	wFM [-421.437048]
2d	-421.556915	AFM [-421.556840]
2e	-420.658462	FM [-420.658491]
2f	-424.495316	NM
2g	-420.670591	wFM [-420.670592]
2h	-421.451182	FM [-421.451221]
2i	-421.867790	AFM [-421.867788]
2j	-421.547371	AFM [-421.605684]
2k	-420.660695	FM [-420.660785]
2l	-420.666614	FM [-420.666601]
2m	-420.657327	FM [-420.657253]
2n	-421.288757	AFM [-421.288678]
2o	-424.497828	NM
2p	-420.713047	FM [-420.713073]
2q	-420.721885	FM [-420.721858]
2r	-420.703455	FM [-420.703466]
4a	-405.263527	wFM [-405.263504]
4b	-405.215841	wFM [-405.215876]
4c	-403.522028	AFM [-403.522042]
4d	-403.448965	FM [-403.449126]
4e	-404.723499	AFM [-404.723498]
8	-383.464713	NM
8a	-374.755651	AFM [-374.756788]
8b	-377.332074	AFM [-377.332003]

[a] The total energies of optimized surface defected GeNWs.
[b] The FM, wFM, AFM and NM indicate the ferromagnetic, weak ferromagnetic, anti-ferromagnetic and non-magnetic respectively.
[c] The value in the parentheses are the total energies of FM or AFM surface defected GeNWs.

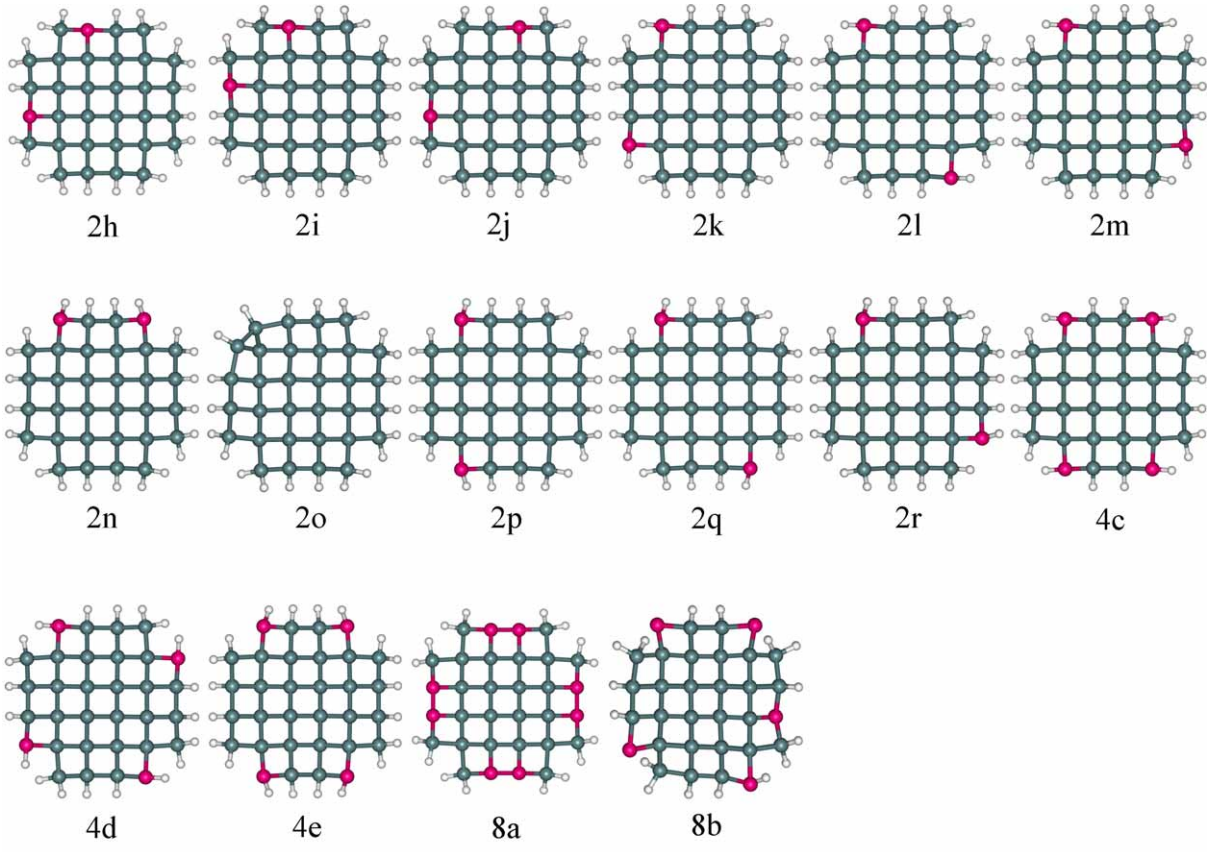

Figure S3 The optimized structures of surface defected GeNWs. Green sphere – Ge, pink sphere – Ge with SDB and white sphere – H.

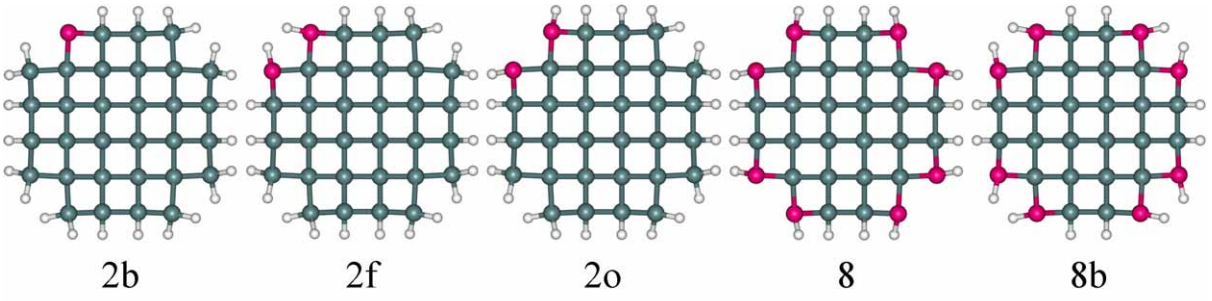

Figure S4 The initial structures of GeNWs undergo surface reconstruction.

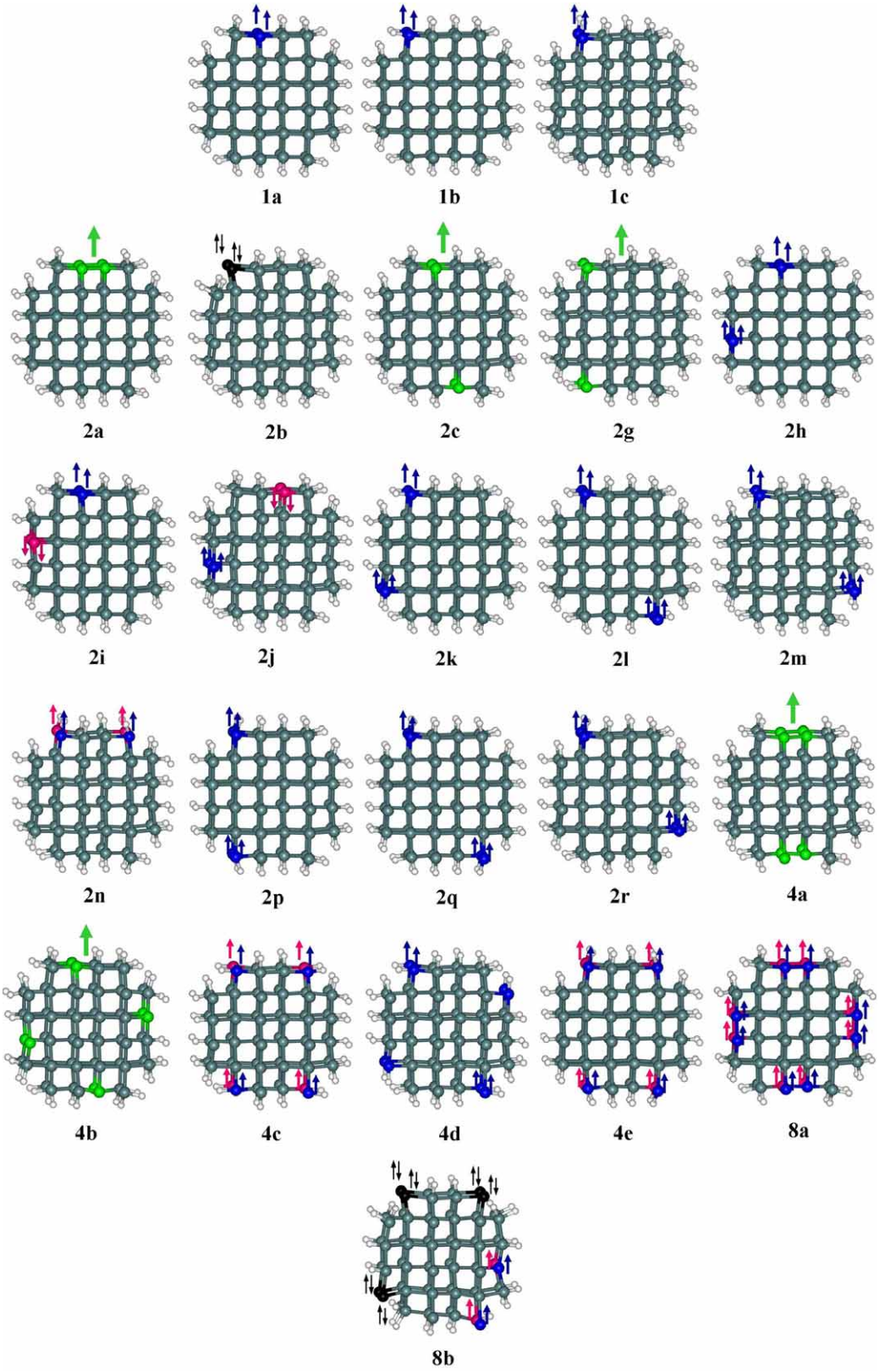

Figure S5 The electron configurations in surface defected GeNWs. The blue and pink spheres indicate the spin-up and spin-down, respectively. The black sphere indicates the singlet-state. The blue sphere indicates the weak ferromagnetic.

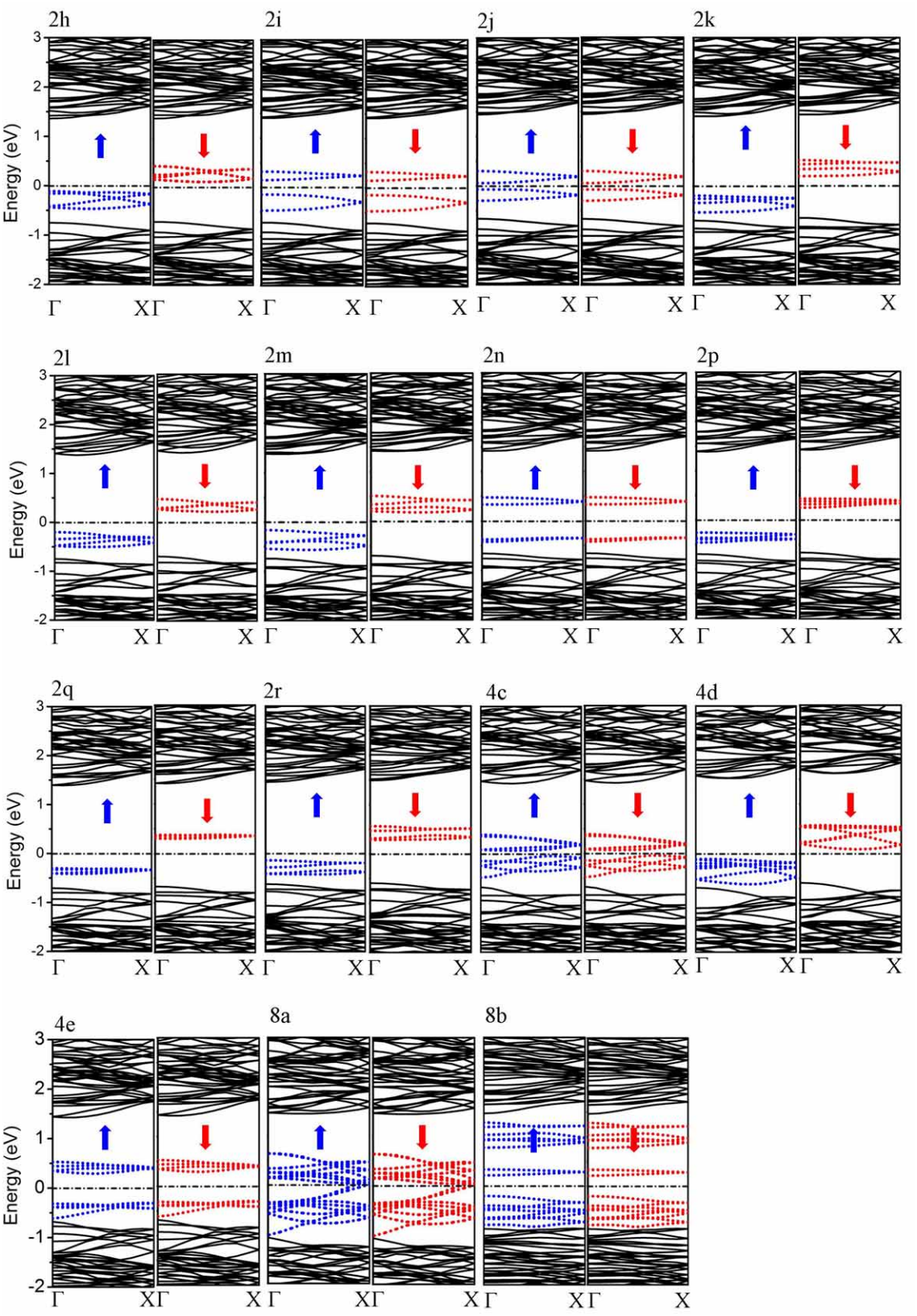

Figure S6 Band structures of surface defected GeNWs. The band structure of **2o** is same with **2f** and not shown here.

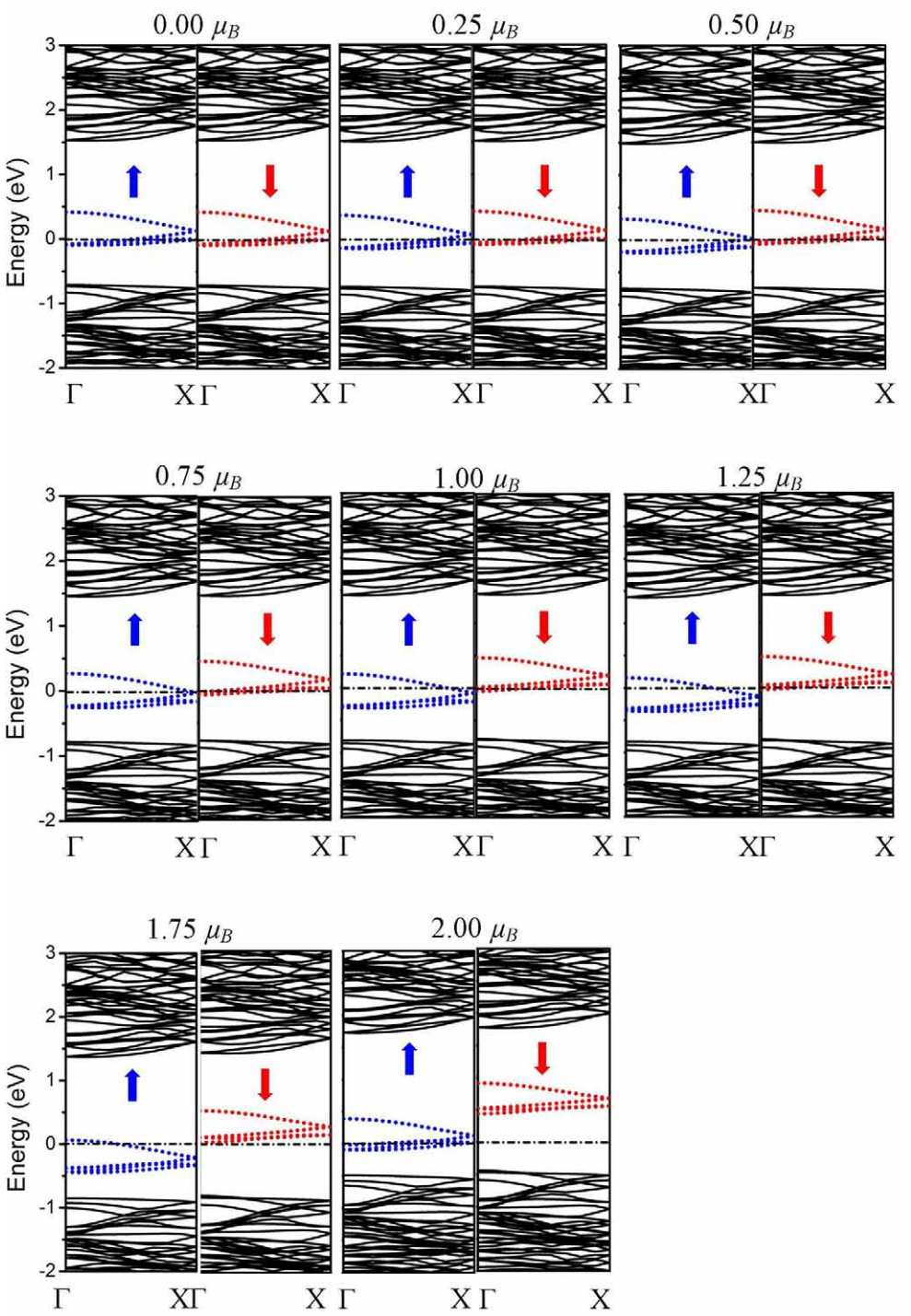

Figure S7 The band structures of **2c** with different magnetic moments. The net magnetic moments are shown on top.