Supplemental information for "Spin reorientation in antiferromagnetic Dy_2FeCoO_6 double perovskite"

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Density functional theory results

The total density of states (DOS) for AFM2 order with and without spin orbit coupling (SOC) are found to be metallic, which is shown in figure S1. Then, we apply electron correlation and SOC simultaneously, which shows band gap values of 1.77 eV and 1.74 eV under GGA + U and GGA + U + SOC scheme respectively, which are insulating. After applying Coulomb interaction (U), Dy-4f, Fe-3d and Co-3d bands move outward from the Fermi level. But by analysing SOC effect we considered GGA + SOC and GGA + U + SOC, SOC alone can not open the gap. However, SOC with electron-correlation, the value of band gap decreases slightly and spin magnetic moments remain the same, which means that the SOC is not influencing this particular system as shown in Table S1. The DOS and band structures are shown in figure S1, figure S2 and figure S3.

Figure S4 represents the partial DOS of t_g and e_{2g} levels of Fe and Co, under GGA + U functionals. When we apply SOC over GGA, the ground state is found along the 111-direction with the second competitive direction 010-direction with an energy difference of 11.39 meV/f.u.. Similarly, under GGA + U + SOC, ground state is found in the 010-direction with competitive 111-direction of an energy difference of 10.56 meV/f.u.. This difference in the direction is due to the presence of Dy-atom. So, we replaced all Dy atoms with La to form La_2FeCoO_6 and performed the same calculations and found that the ground state is in 010-direction under both GGA + SOC and GGA + U + SOC, which are tabulated in Table S1. The other properties spin magnetic moment, orbital magnetic moment and band gap of Dy_2FeCoO_6 and La_2FeCoO_6 are comparable, which shows similar nature which are tabulated in Table S2 and Table S3 respectively. The double perovskite Dy_2FeCoO_6 is an AFM, in which Fe and Co are antiparallel to each other and the total magnetic moment is zero. But Dy also contributes larger spin and orbital magnetic moments and this compound contains four Dy atoms, in which three are in one direction and one is opposite to others, so the total magnetic moment is contributed by two Dy atoms only. The value of the total magnetic moment is equal to 10 μ_B under GGA + U calculation. Further, to check the effect of Dy on Fe and Co, we replaced Dy by La and found that the value of spin magnetic moment is zero. From the ground state energy in AFM2-configuration, Fe and Co are found to align antiparallel, hence the total magnetic moment is equal to zero.

In Dy_2FeCoO_6, the atomic spin magnetic moments are found to be 4.97 μ_B per Dy, $\pm$4.10 μ_B per Fe and $\mp$ 0.18 μ_B per Co and their corresponding orbital magnetic moments are 1.98 μ_B, 0.01 μ_B and 0.02 μ_B respectively as shown in Table S2. Depending upon the positions of atoms, oxygen gains small magnetic moment due to hybridizations with Dy-4f, Fe-3d and Co-3d.
From the DOS and band structure plots, we can see that there are only few bands that are crossing at the Fermi level, due to which the system shows metallic nature.

This band opens up a large gap after applying the Coulomb interaction, which shows direct band gap at M-symmetry point (refer figure S5 and figure S6). The variation of electronic band gap of Dy_2FeCoO_6 with different U values of Fe and Co is shown in figure S7. The band gap is found to increase with the electron correlations of Fe and Co.

Table S1. Calculated spin magnetic moments (in μ_B) of Fe-3d, Co-3d and band gap (in eV). The calculated orbital moments are shown within parentheses for La_2FeCoO_6.

	Fe	Co	Band gap (eV)
GGA	3.47	0.45	Metallic
GGA+SOC	3.47	0.45	0.08
	(0.03)	(0.04)	
GGA+U	4.07	0.18	1.49
GGA+U+SOC	4.06	0.18	1.54
	(0.01)	(0.02)	

Table S2. Relative total energies (in meV/f.u.) calculated within GGA functional for Dy_2FeCoO_6 and La_2FeCoO_6.

	FM	AFM1	AFM2	FIM1	FIM2	FIM3
Dy_2FeCoO_6	144.67	10.40	0	143.23	13.23	155.66
La_2FeCoO_6	167.18	235.53	0	167.17	235.54	167.19

Table S3. Relative total energies (in meV/f.u.) calculated within GGA + SOC and GGA + U + SOC functional for Dy_2FeCoO_6 and La_2FeCoO_6 in five posible directions.

	100	010	001	110	111
GGA + SOC [Dy_2FeCoO_6]	28.87	11.39	45.97	20.47	0
GGA + U + SOC [Dy_2FeCoO_6]	46.79	0	47.44	44.52	10.56
GGA + SOC [La_2FeCoO_6]	0.47	0	0.57	0.20	0.35
GGA + U + SOC [La_2FeCoO_6]	0.66	0	0.50	0.23	0.33

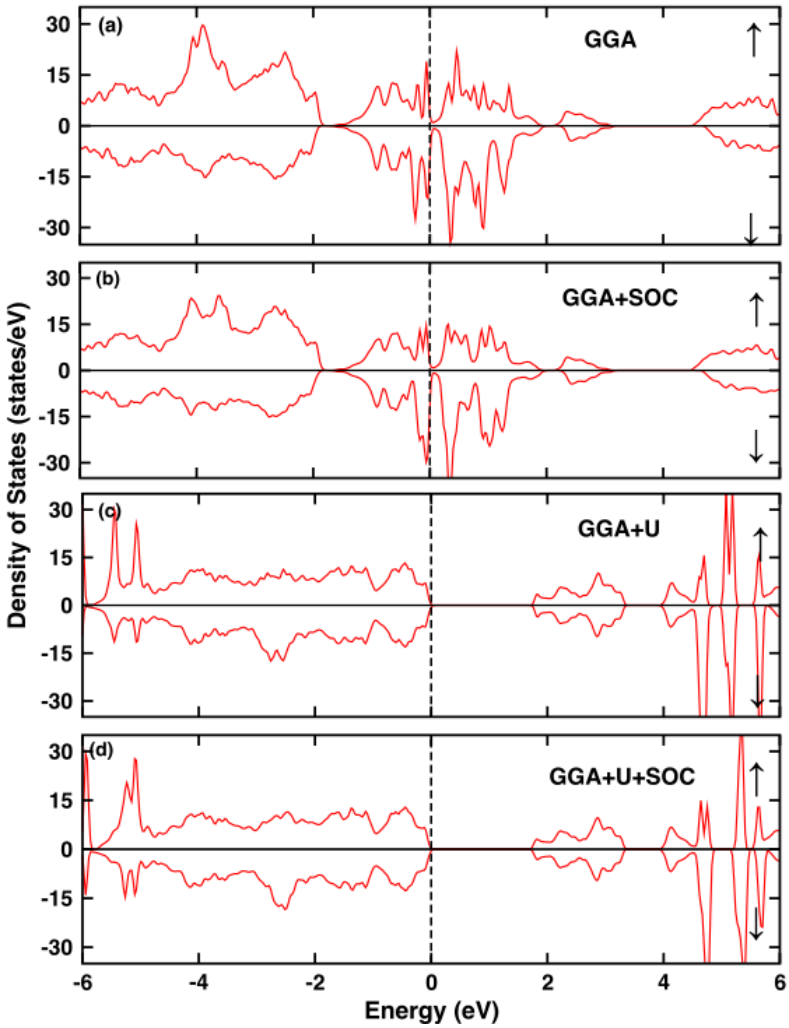

Figure S1. (color online) Total DOS of the Dy_2FeCoO_6 for (a) GGA, (b) GGA + SOC, (c) GGA + U and (d) GGA + U + SOC functionals in spin up (↑) and spin down (↓) channel. The vertical dotted line indicates $E_F = 0$.

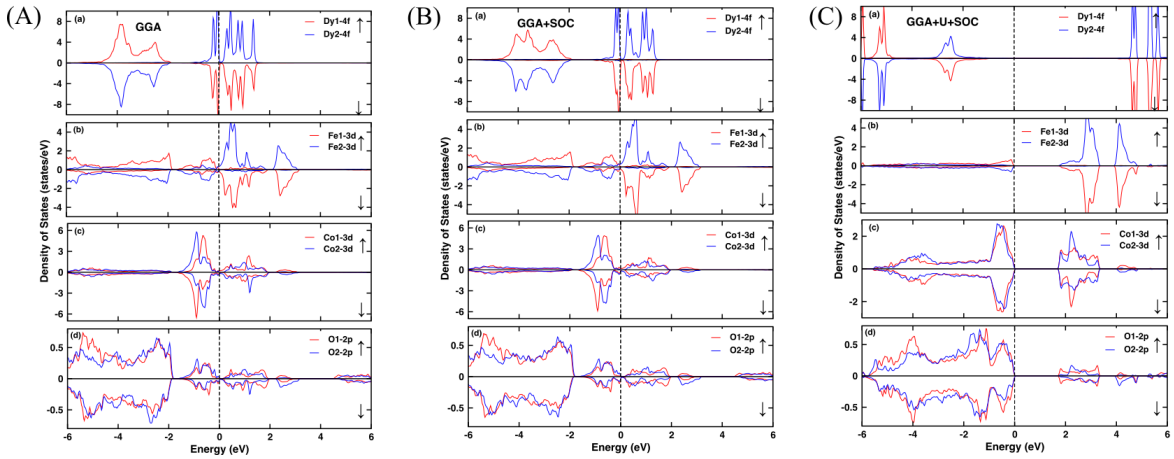

Figure S2. (color online) Partial DOS of (a) Dy-4f (b) Fe-3d (c) Co-3d and (d) O-2p in spin up (↑) and spin down (↓) channel for GGA (left), GGA + SOC (middle) and GGA + U + SOC (right). The vertical dotted line indicates $E_F = 0$.

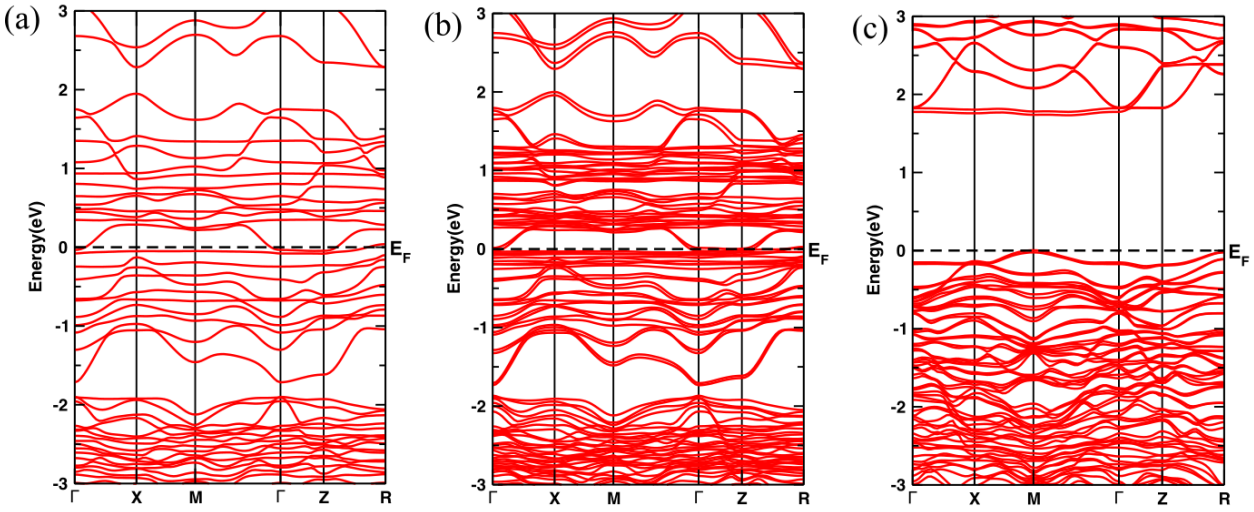

Figure S3. (color online) Band structures within (a) GGA, (b) GGA + SOC and (c) GGA + U + SOC. Dashed horizontal lines at zero energy corresponds to the Fermi level.

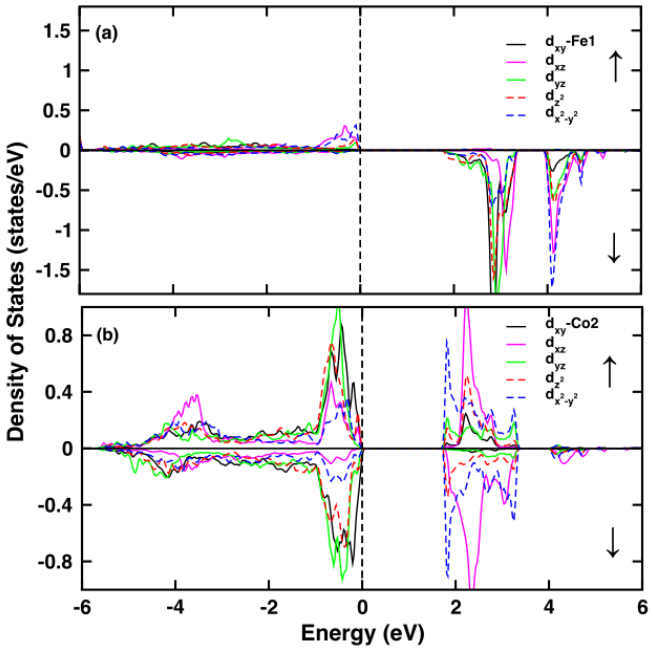

Figure S4. (color online) Partial DOS of (a) Fe-3d and (b) Co-3d for e_g [$d_{z^2} + d_{x^2y^2}$] (dotted lines) and t_{2g} [$d_{xy} + d_{xz} + d_{yz}$] (solid lines) under GGA + U functionals. The vertical dotted line indicates $E_F = 0$.

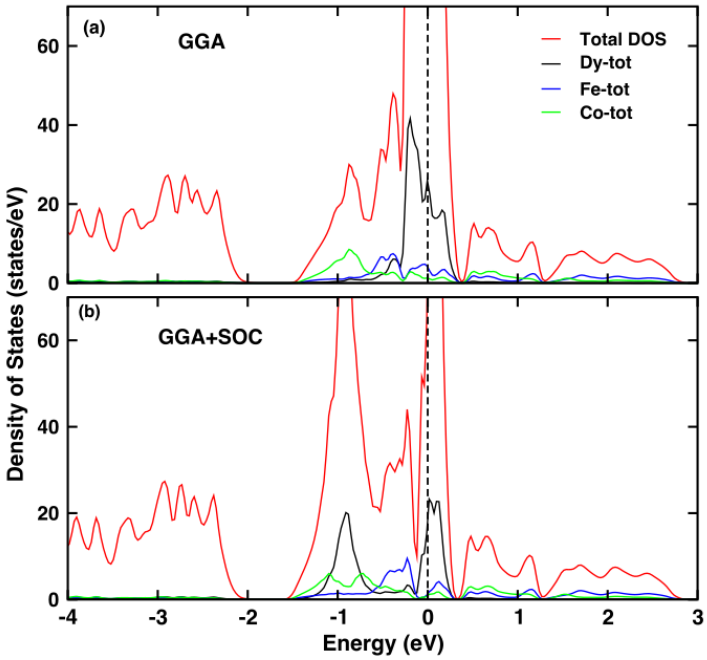

Figure S5. (color online) Total and partial DOS of the Dy_2FeCoO_6 under (a) GGA and (b) GGA + SOC functionals for non-magnetic calculation. The vertical dotted line indicates $E_F = 0$.

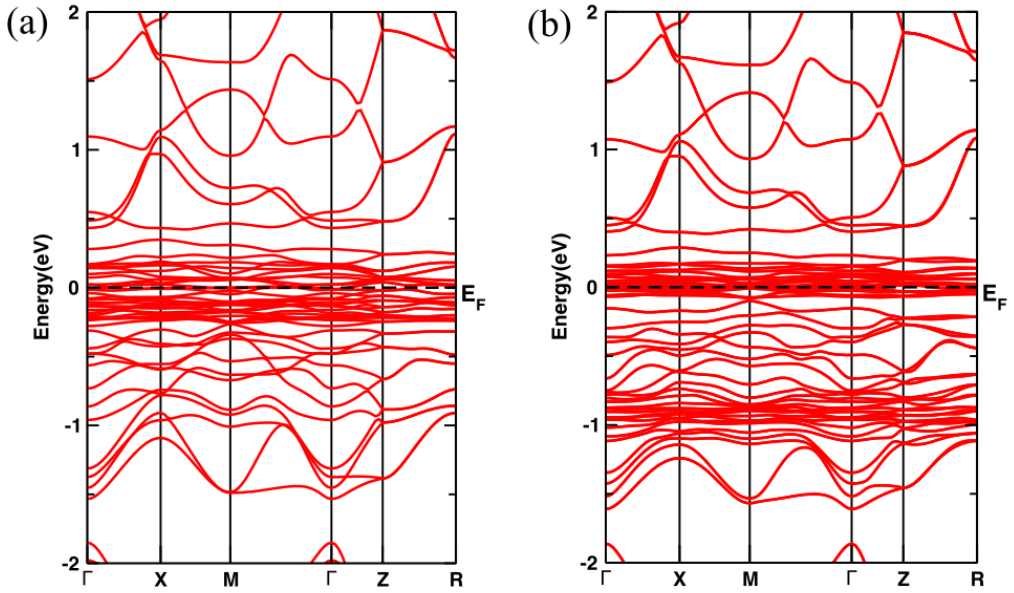

Figure S6. (color online) Band structures within (a) GGA and (b) GGA + SOC for non-magnetic calculation. Dashed horizontal lines at zero energy corresponds to the Fermi level.

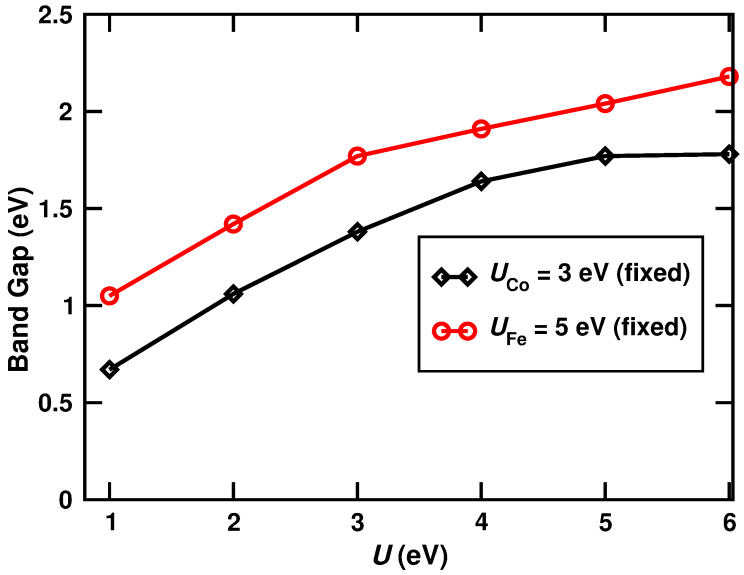

Figure S7. (color online) Variation of band gap with the effects of electron correlations (U). Here the U value for Dy is fixed to 7 eV.