

1 Spinel CoFe_2O_4 : Room temperature magnetic semiconductor with optical 2 transparency

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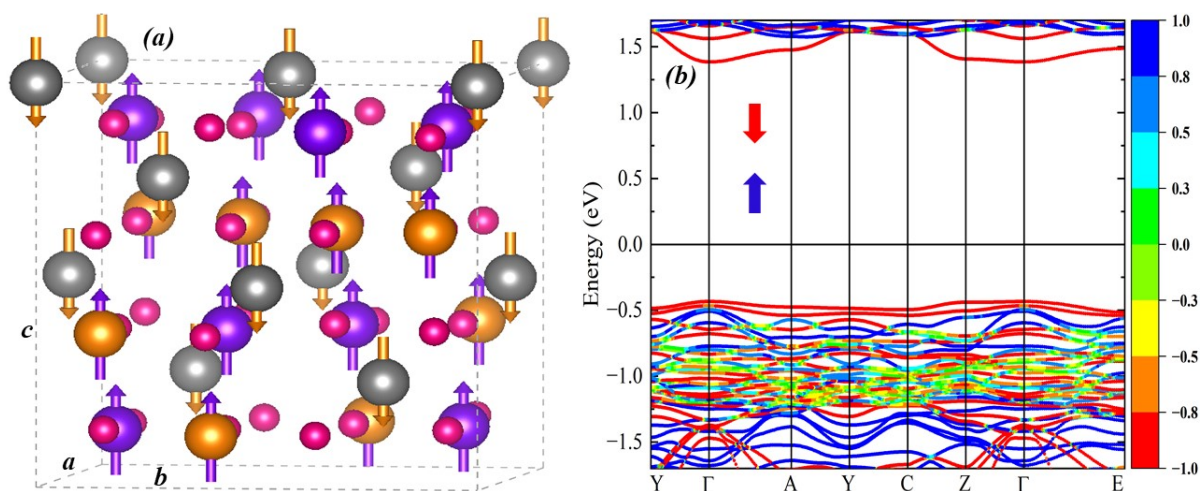
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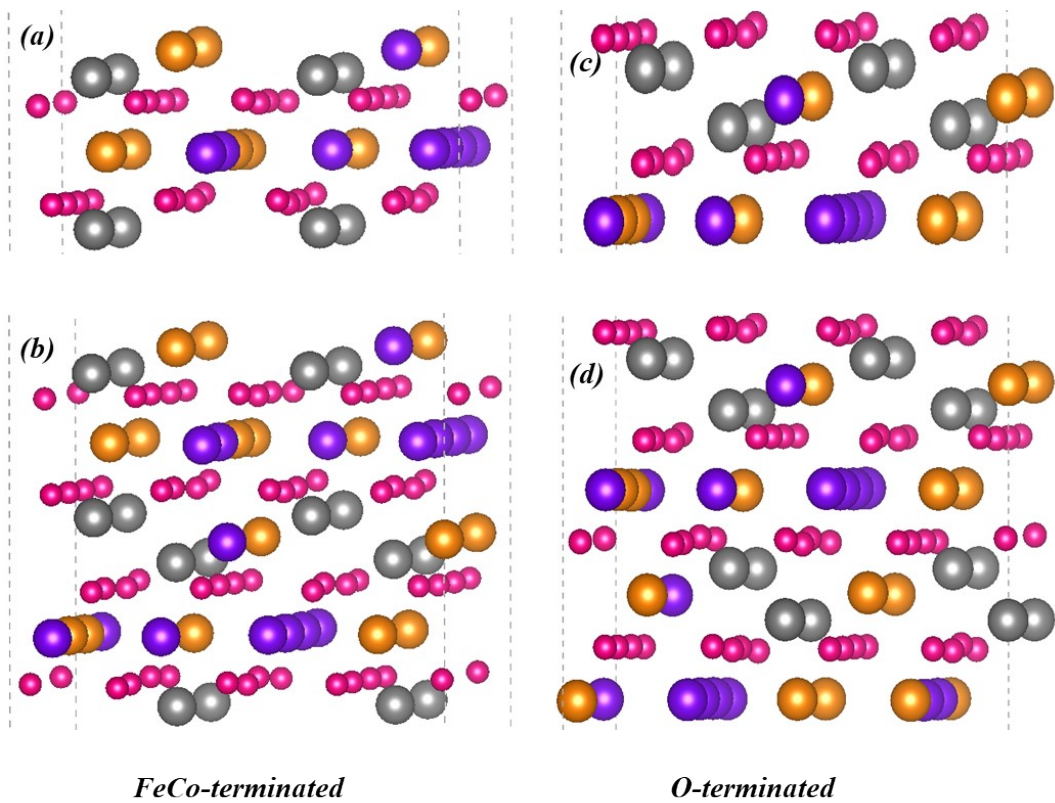
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10 Supporting information



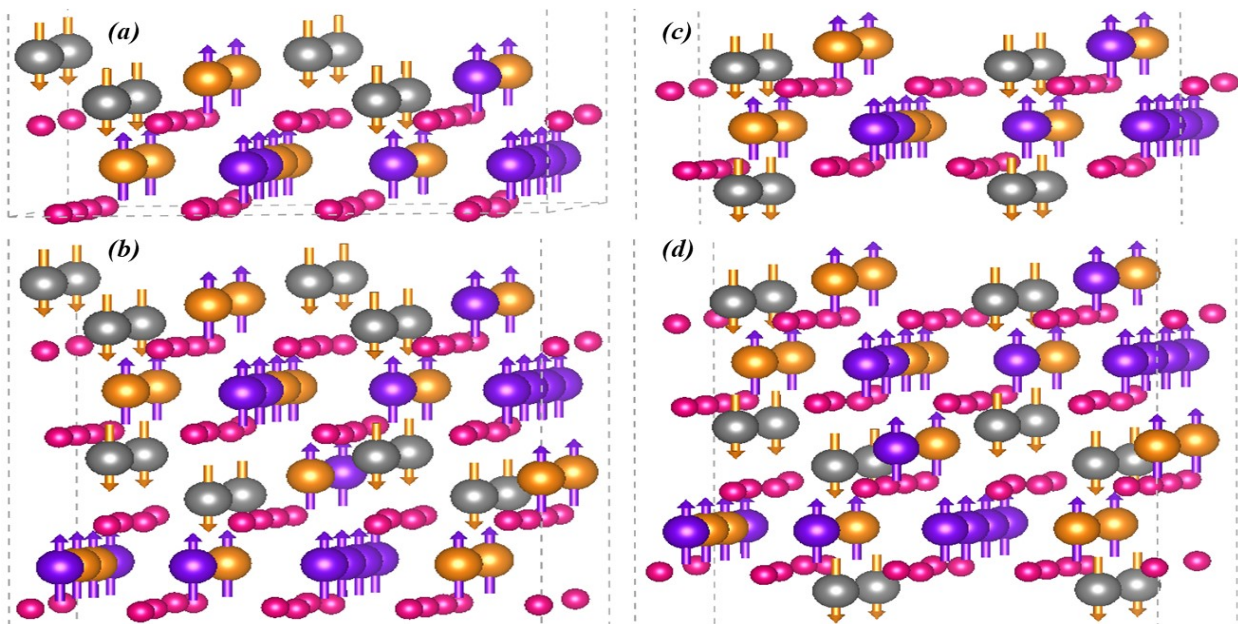
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15 **Figure S1.** (a) Ferrimagnetic configurations and (b) spin-projected band structure including SOC in bulk CFO.



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17 **Figure S2.** Crystal structures of (a) FeCo-terminated 1UC, (b) FeCo-terminated 2UC, (c) O-terminated 1UC, and O-
 18 terminated 2UC CFO systems.

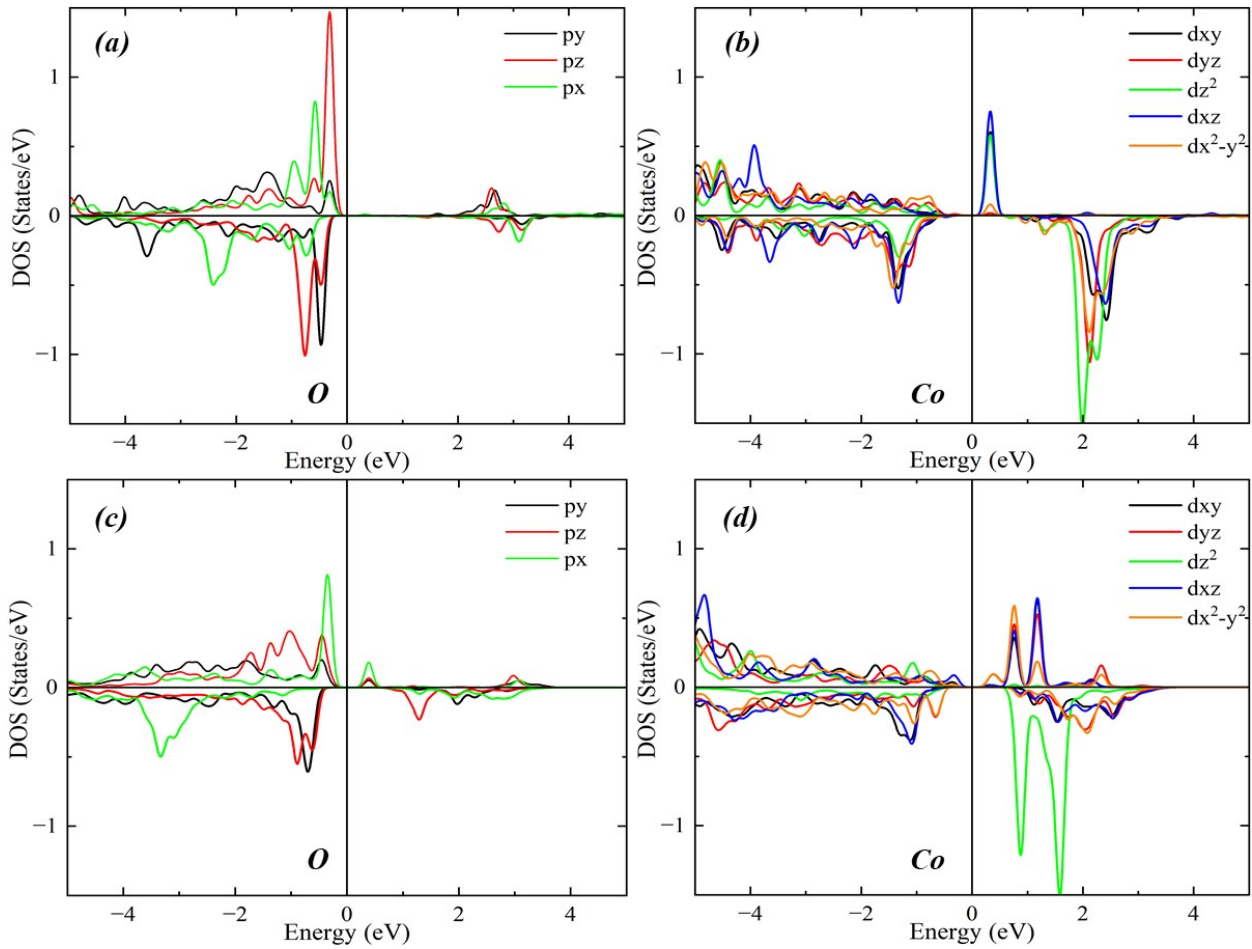
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21 **Figure S3.** Ferrimagnetic configurations in Fe-terminated (a) 1UC, (b) 2UC, FeCo-terminated (c) 1UC, and (d) 2UC
 22 thin films.

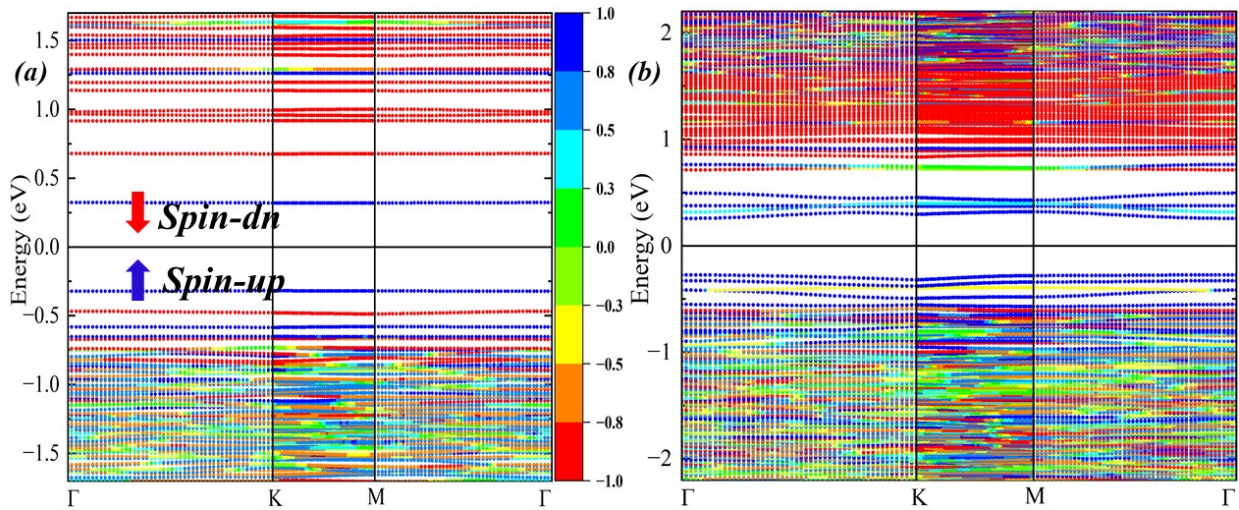
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25 **Figure S4.** Spin-polarized (a) partial density of states of O in 1UC, (b) partial density of states of Co in 1UC, (c) partial
 26 density of states of O in 2UC, (d) partial density of states of Co in 2UC with Fe-terminations.

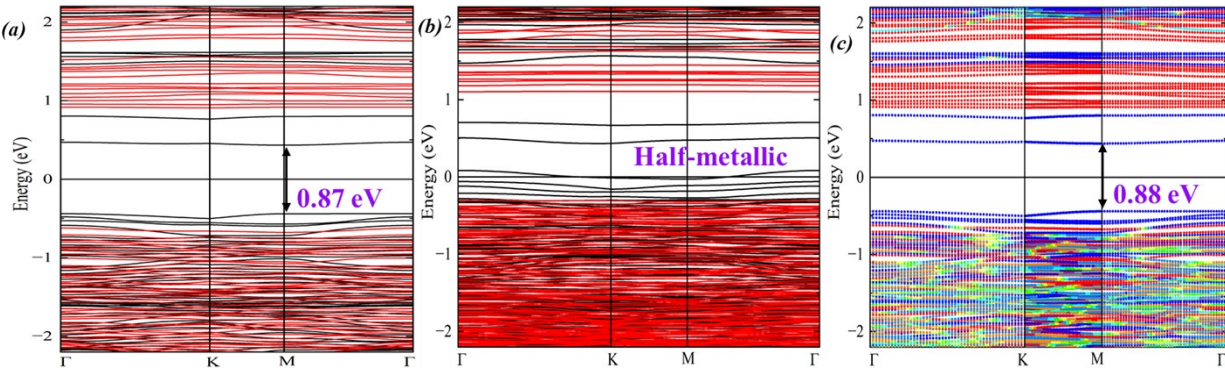
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29 **Figure S5.** Spin projected band structure after including the SOC (a) 1UC, and (b) 2UC CFO structures with Fe-
 30 terminations.

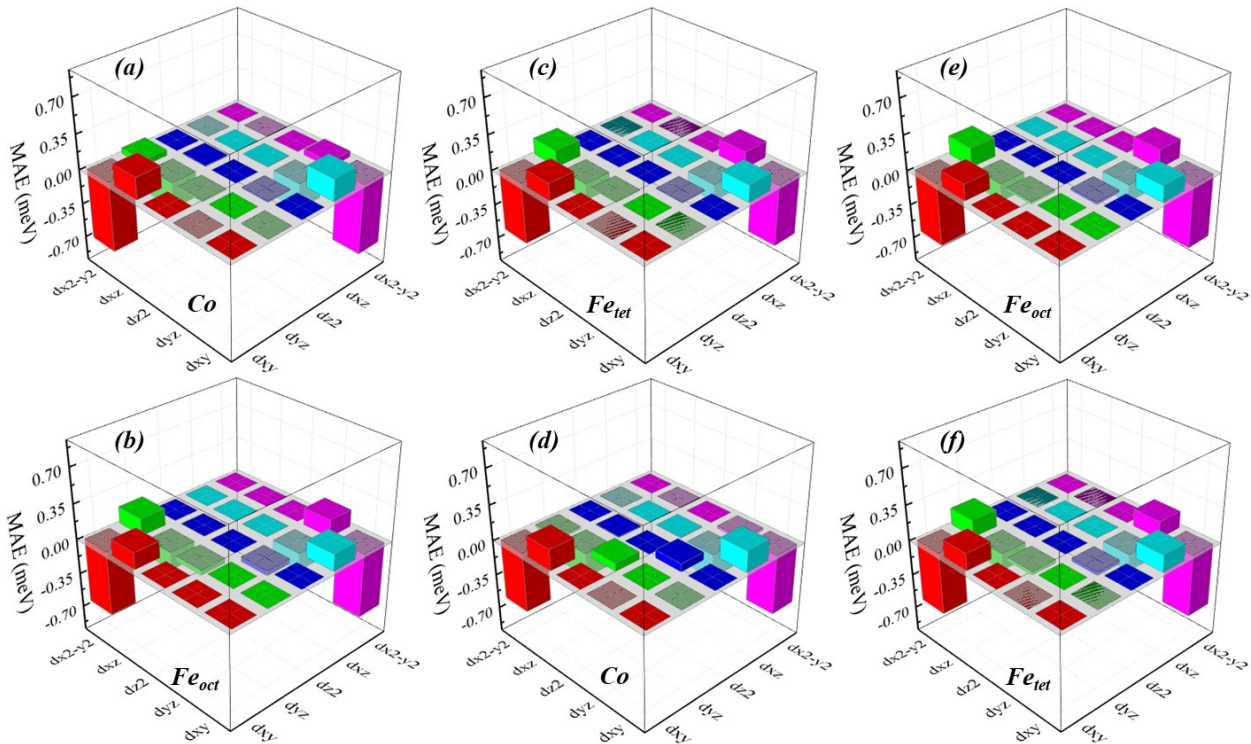
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33 **Figure S6.** Band structure of (a) 1UC, (b) 2UC without SOC, and (c) 1UC with SOC in FeCo-termination.

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36 **Figure S7.** SOC matrix analysis of (a) – (c) Co, Fe_{oct}, and Fe_{tet} in 1UC thin film, and (d) – (f) Co, Fe_{oct}, and Fe_{tet} in 2UC
 37 thin film with FeCo-termination.

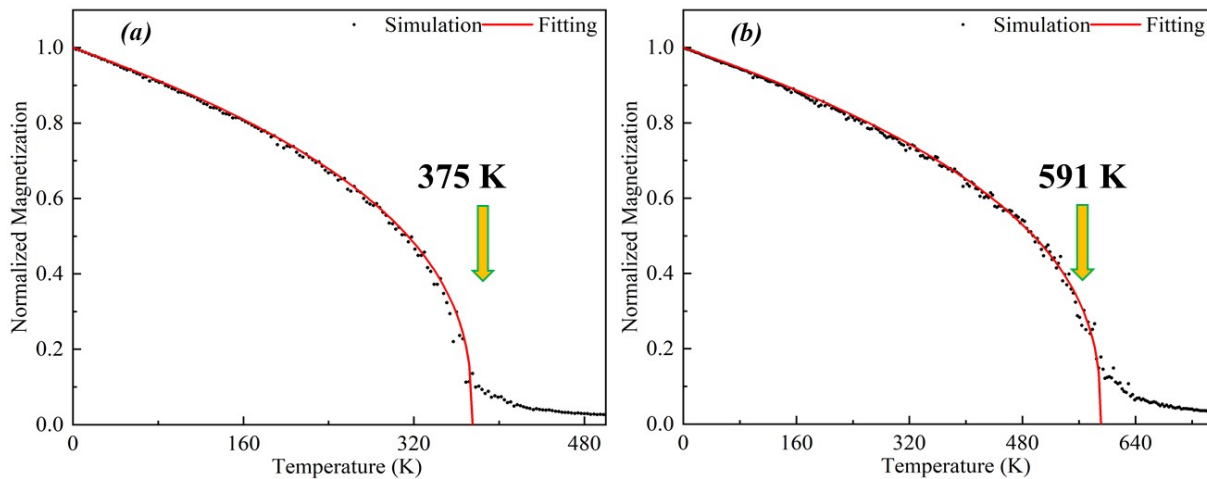
38 Figure S7 (a) – (f) in the SI illustrates the SOC matrix elements of the Co, Fe_{oct}, and Fe_{tet} atoms in 1UC and 2UC CFO
 39 with FeCo-termination. Here the positive and negative values correspond to contributions to the out-of-plane and
 40 in-plane MAE. In all the atoms of both thin film systems, the dominant contribution to the in-plane MAE comes from
 41 the SOC in the ($d_{x^2-y^2} - d_{xy}$) orbitals. The SOC between ($d_{xz}-d_{xy}$) on the other hand produces a small out-of-plane
 42 contribution also. Nonetheless, the in-plane contribution dominated and we found in-plane anisotropy of -169
 43 $\mu\text{eV}/\text{atom}$ and -84 $\mu\text{eV}/\text{atom}$ in both systems respectively.

44 **Table S1** Exchange interaction (J), single-ion magnetic anisotropy (k_2), magnetic moment (m_2), and Curie temperature
 45 (T_C) in bulk and thin film CFO structures.

Systems/parameters	J ($\times 10^{-21}$ J)	k_2 ($\times 10^{-24}$ J)	m_2 (μ_B)	T_C (K)
Bulk CFO	3.63	-5.54	2.67	843
Fe-terminated 1UC	2.71	-9.55	2.82	471
Fe-terminated 2UC	3.43	-14.6	2.48	582
FeCo-terminated 1UC	2.18	-27.04	2.77	375
FeCo-terminated 2UC	3.48	-13.5	2.69	591

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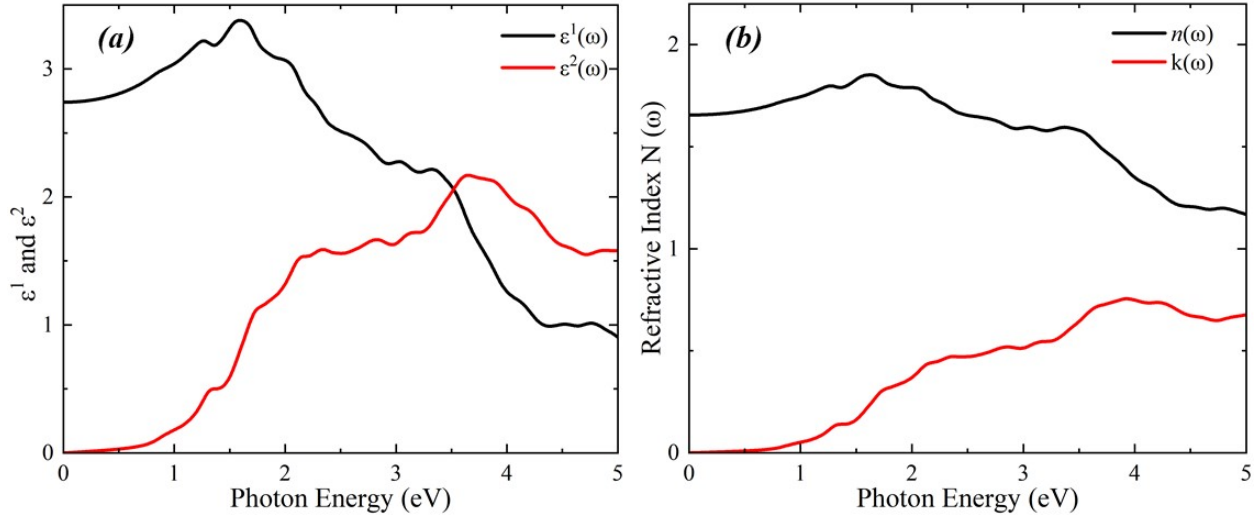
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49 **Figure S8.** Temperature-dependent magnetization curve for (a) 1UC, and (c) 2UC systems with FeCo-termination.

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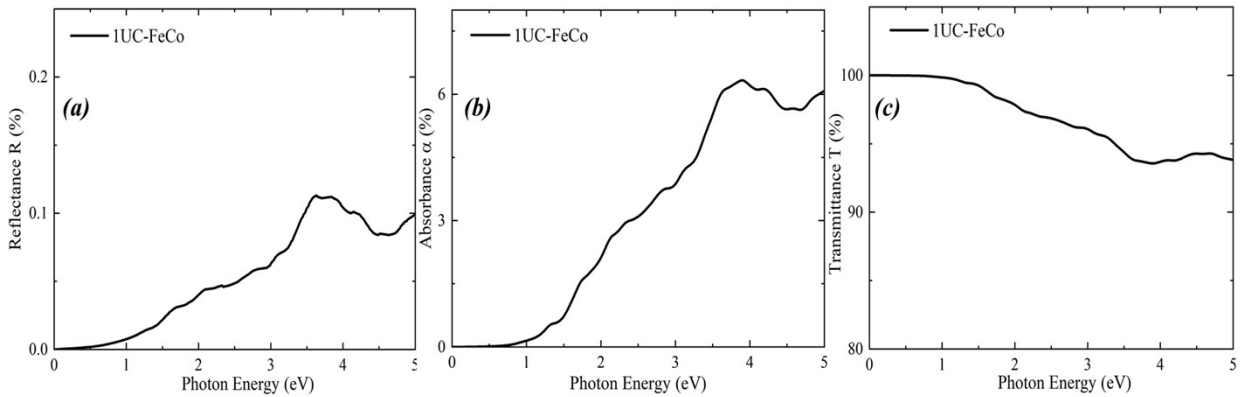
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52 **Figure S9.** (a) The real and imaginary part of the dielectric function and (b) refractive index of 1UC CFO thin film with
53 FeCo-termination.

54

55 Figure S9 (a) shows the real and imaginary part of the frequency-dependent dielectric function for 1UC CFO thin film
56 with FeCo-termination, where the onset of the imaginary part shows the semiconducting nature. Besides, 1UC CFO
57 thin film has a maximum refractive index of 1.78 as shown in Fig. S9 (b).

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60 **Figure S10.** (a) Reflectance (b) absorbance, and (c) transmittance for pristine 1UC thin films with FeCo-termination.

61 Figure S10 (a) shows that the 1UC structure has a very weak reflectance ($\sim 0.06\%$) in visible range. Similarly, the
62 absorbance is also not that high ($\sim 3.7\%$) as shown in Fig. S10 (b). Consequently, the 1UC with FeCo-termination is
63 also optically transparent because the transmittance is more than 96% in the visible frequencies.