

Supplementary Material to the article
“Thermoelectric and magnetic properties of
p-type polycrystalline $\text{Cu}_{11}\text{TM}_1\text{Sb}_4\text{S}_{13}$ (TM =
Mn, Fe, Co, Ni)”

1. SEM, EDX and XRD

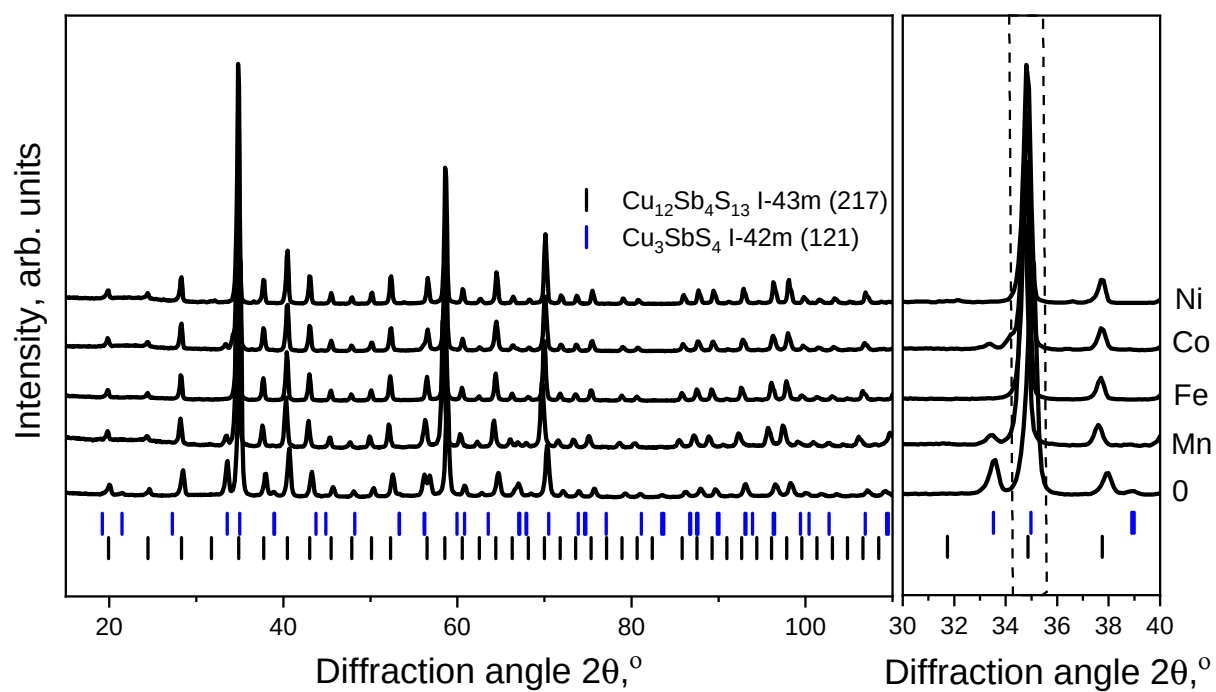


Fig. S1. XRD patterns of all samples

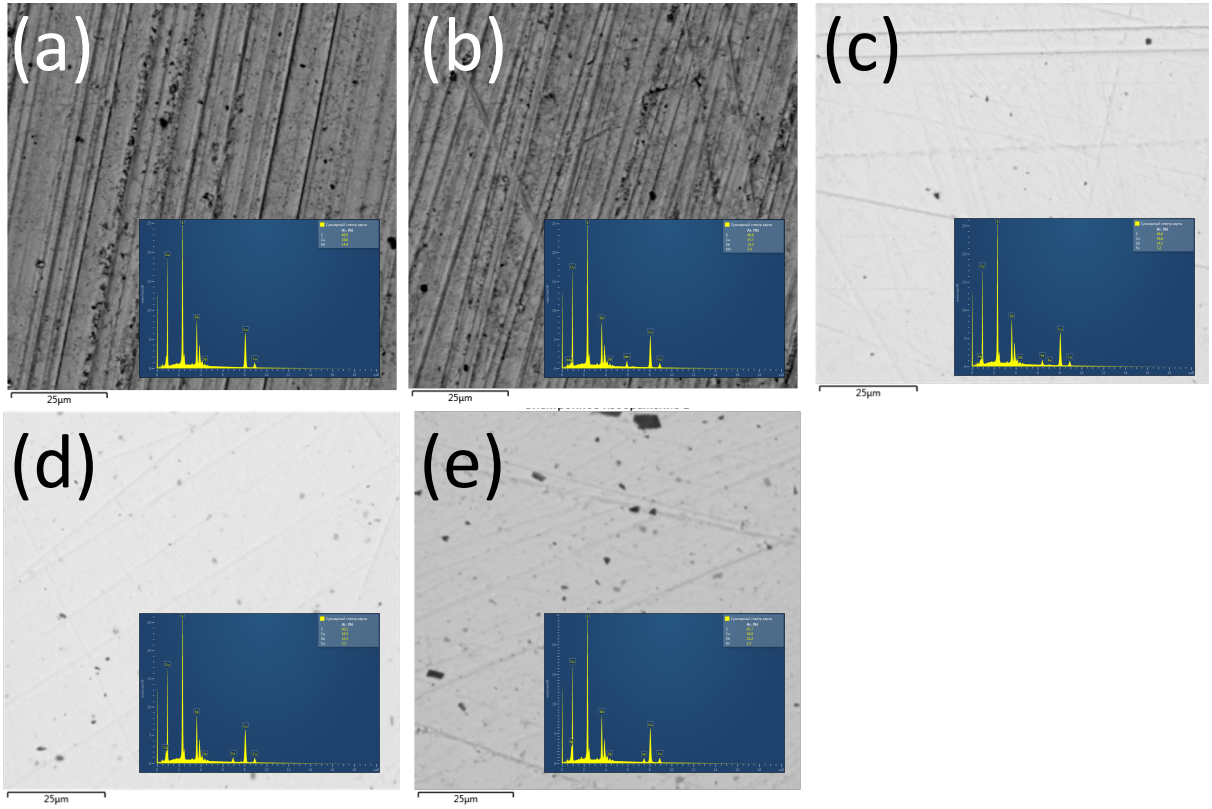


Fig. S2. SEM surface microphotographs and EDX spectra acquired at the same measurement points on the surface for each sample $Cu_{12-x}TM_xSb_4S_{13}$: (a) $x = 0$ (undoped), (b) Mn-substituted, (c) Fe-substituted, (d) Co-substituted, (e) Ni-substituted

2. Mössbauer spectroscopy

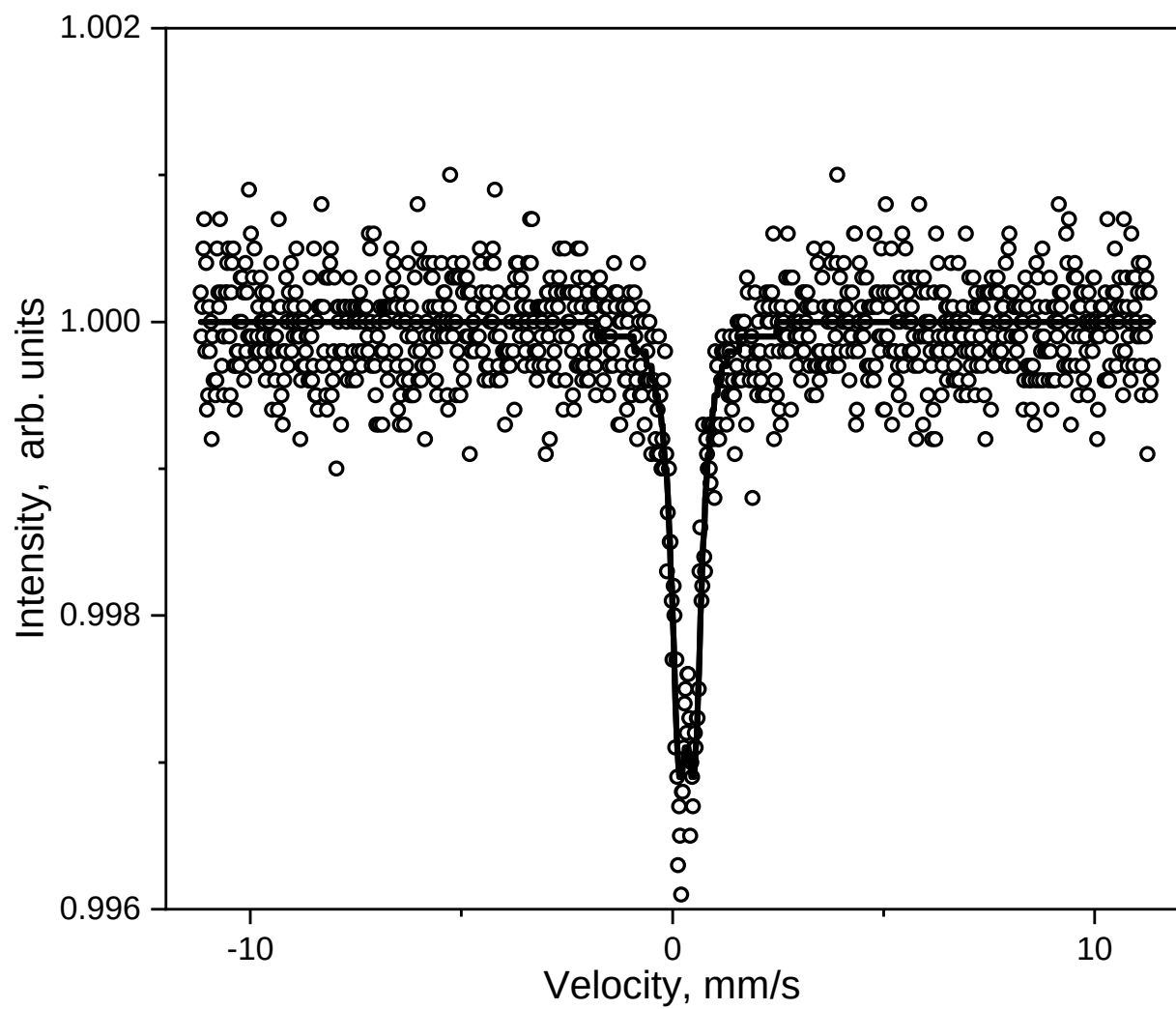


Fig. S3. Mössbauer absorption spectrum of $\text{Cu}_{11}\text{Fe}_1\text{Sb}_4\text{S}_{13}$

3. Band structure of $\text{Cu}_{11}\text{TM}_1\text{Sb}_4\text{S}_{13}$

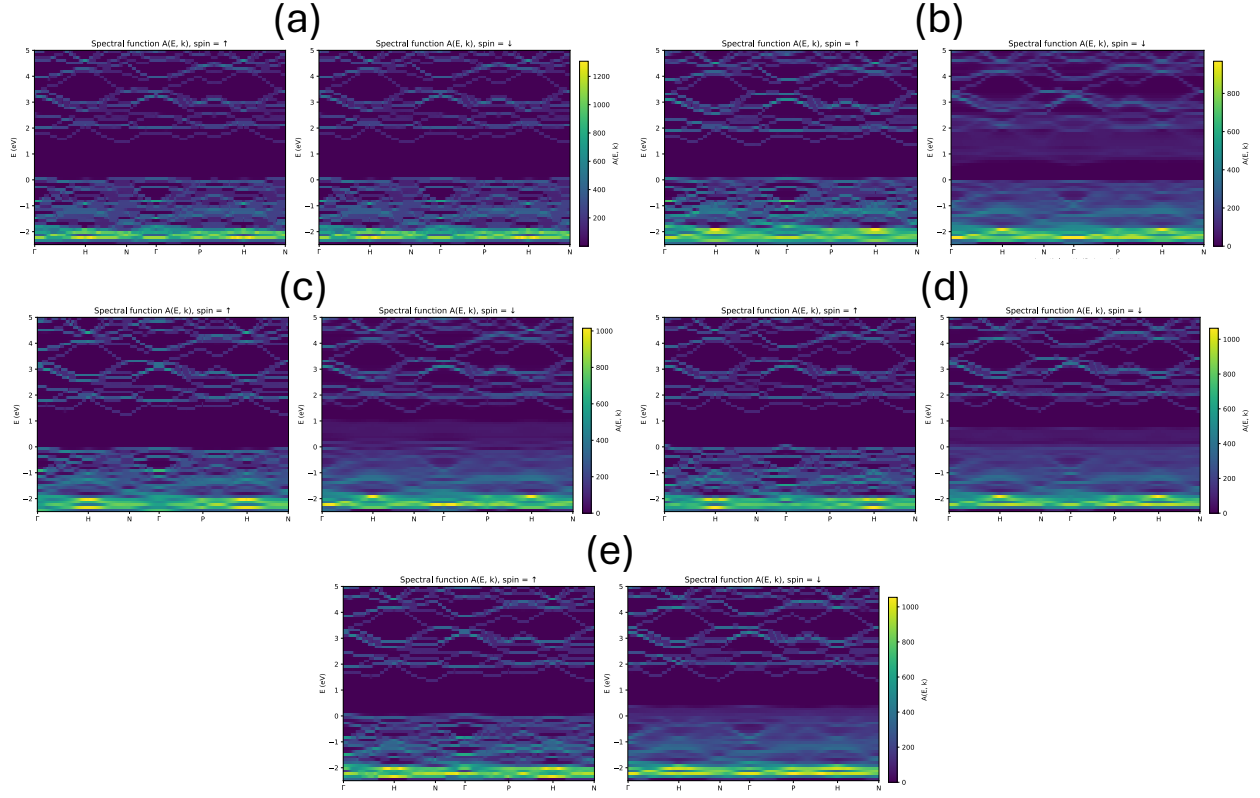


Fig. S4. Electronic structure of $\text{Cu}_{11}\text{TM}_1\text{Sb}_4\text{S}_{13}$: Bloch spectral function $A(\mathbf{k}, \omega)$ obtained from first-principles calculations within the AkaiKKR-CPA formalism for (a) $\text{TM} = 0$ (undoped), (b) Mn, (c) Fe, (d) Co, and (e) Ni. The broadening of the spectral weight reflects the disorder effects arising from substitutional doping on the TM sites

4. pDOS of $\text{Cu}_{11}\text{TM}_1\text{Sb}_4\text{S}_{13}$

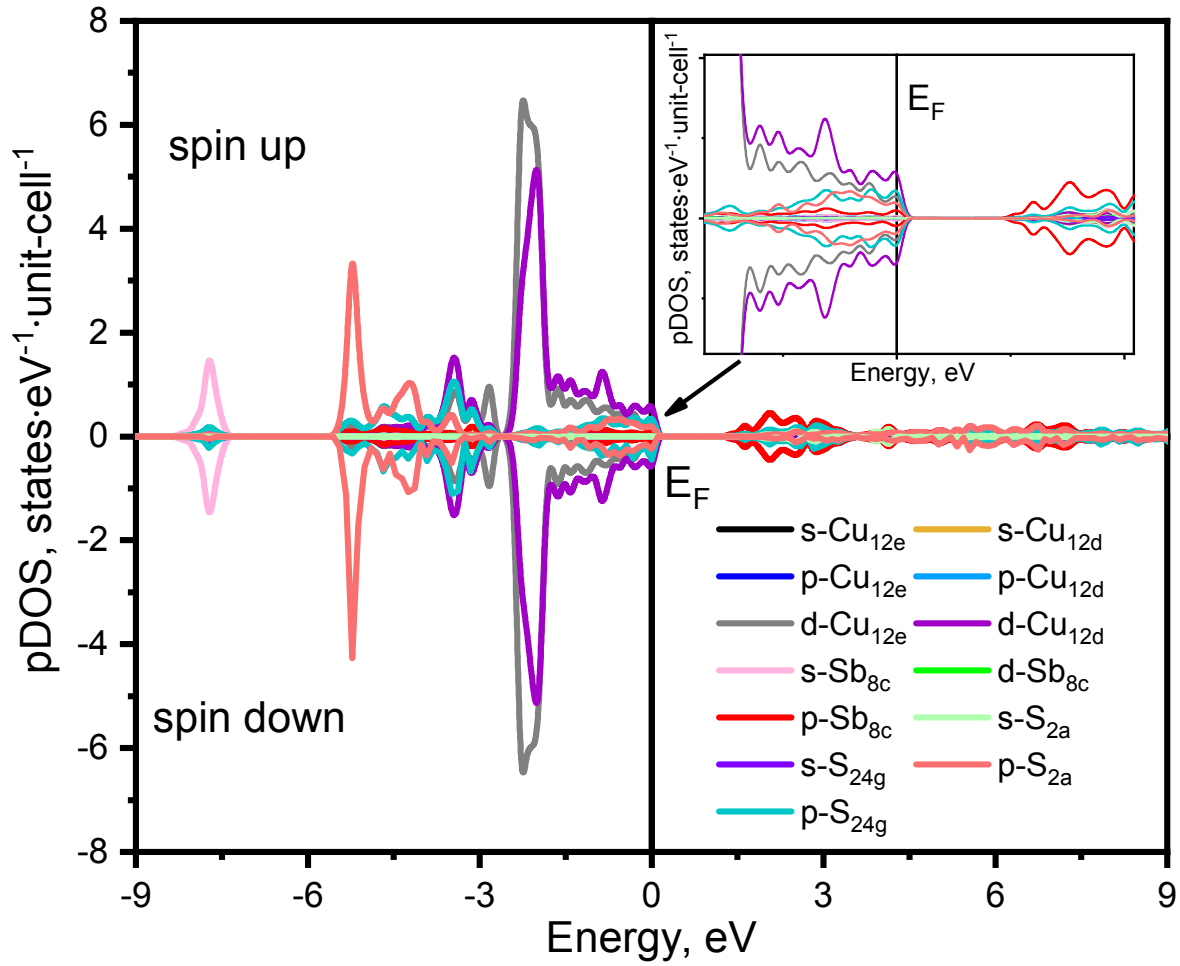


Fig. S5. Spin-polarized pDOS of $\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$ obtained from AkaiKKR-CPA calculations. Vertical line indicates the Fermi level (0 eV)

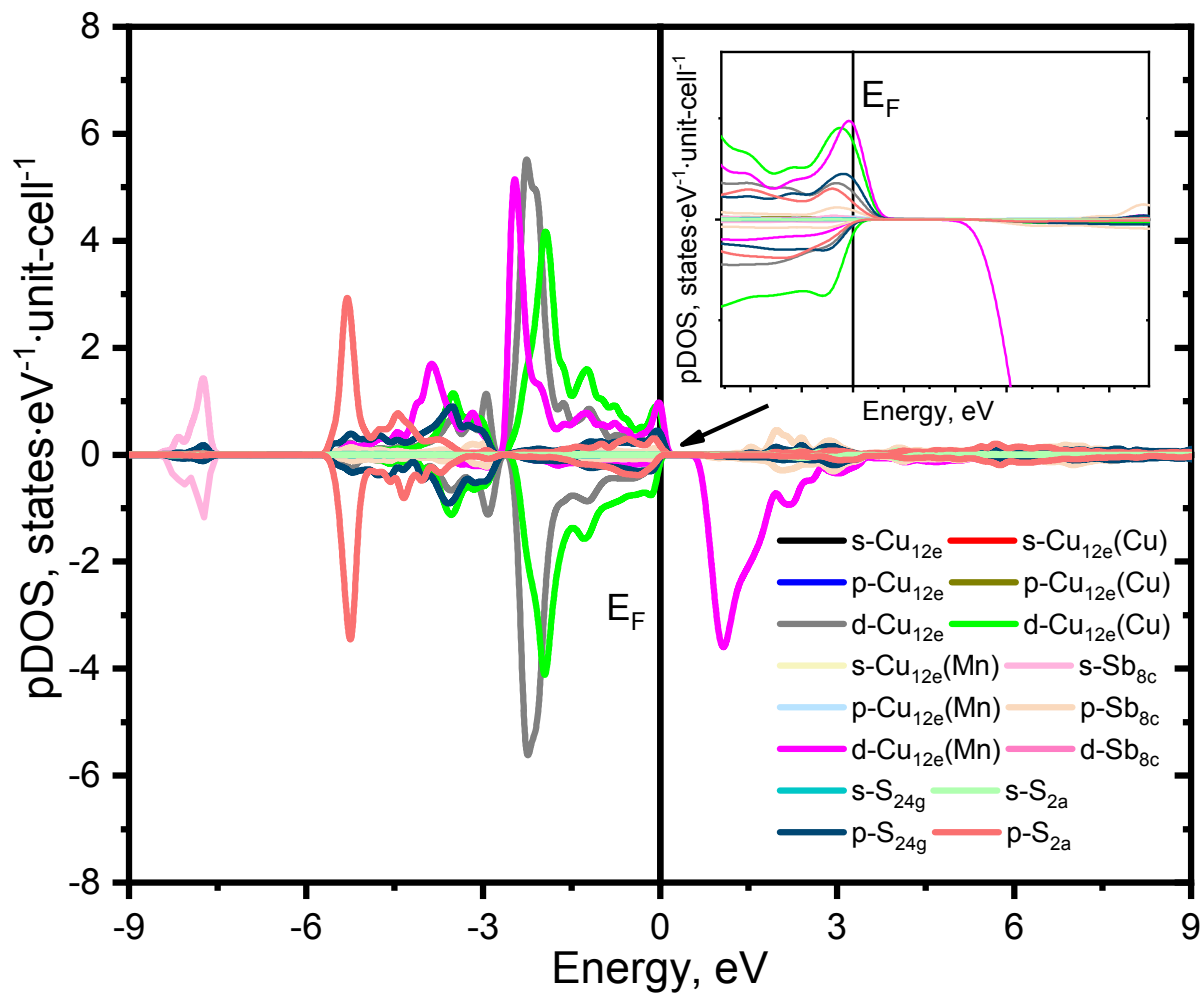


Fig. S6. Spin-polarized pDOS of $\text{Cu}_{11}\text{Mn}_1\text{Sb}_4\text{S}_{13}$ obtained from AkaiKKR-CPA calculations. Vertical line indicates the Fermi level (0 eV)

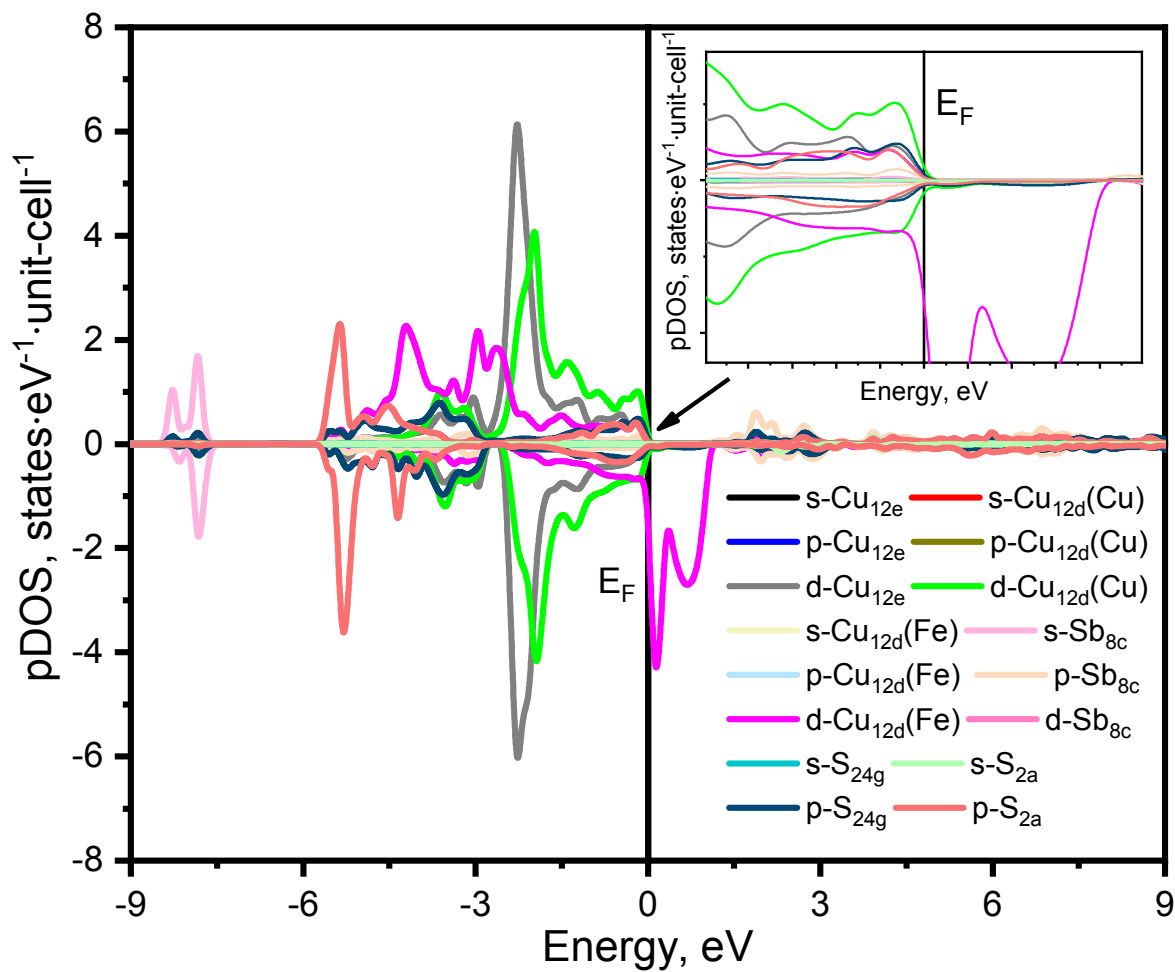


Fig. S7. Spin-polarized pDOS of Cu₁₁Fe₁Sb₄S₁₃ obtained from AkaiKKR-CPA calculations. Vertical line indicates the Fermi level (0 eV)

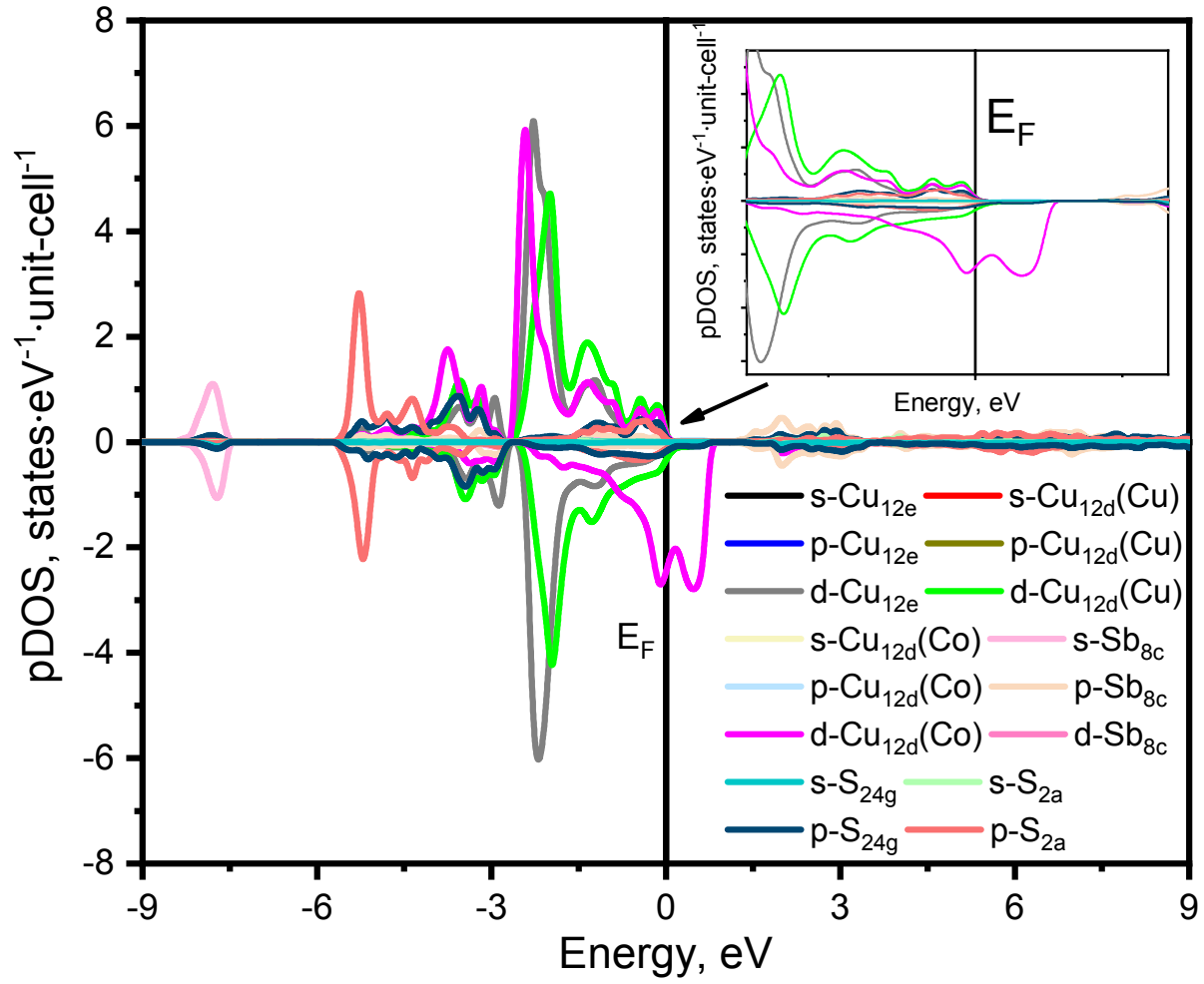


Fig. S8. Spin-polarized pDOS of $\text{Cu}_{11}\text{Co}_1\text{Sb}_4\text{S}_{13}$ obtained from AkaiKKR-CPA calculations. Vertical line indicates the Fermi level (0 eV)

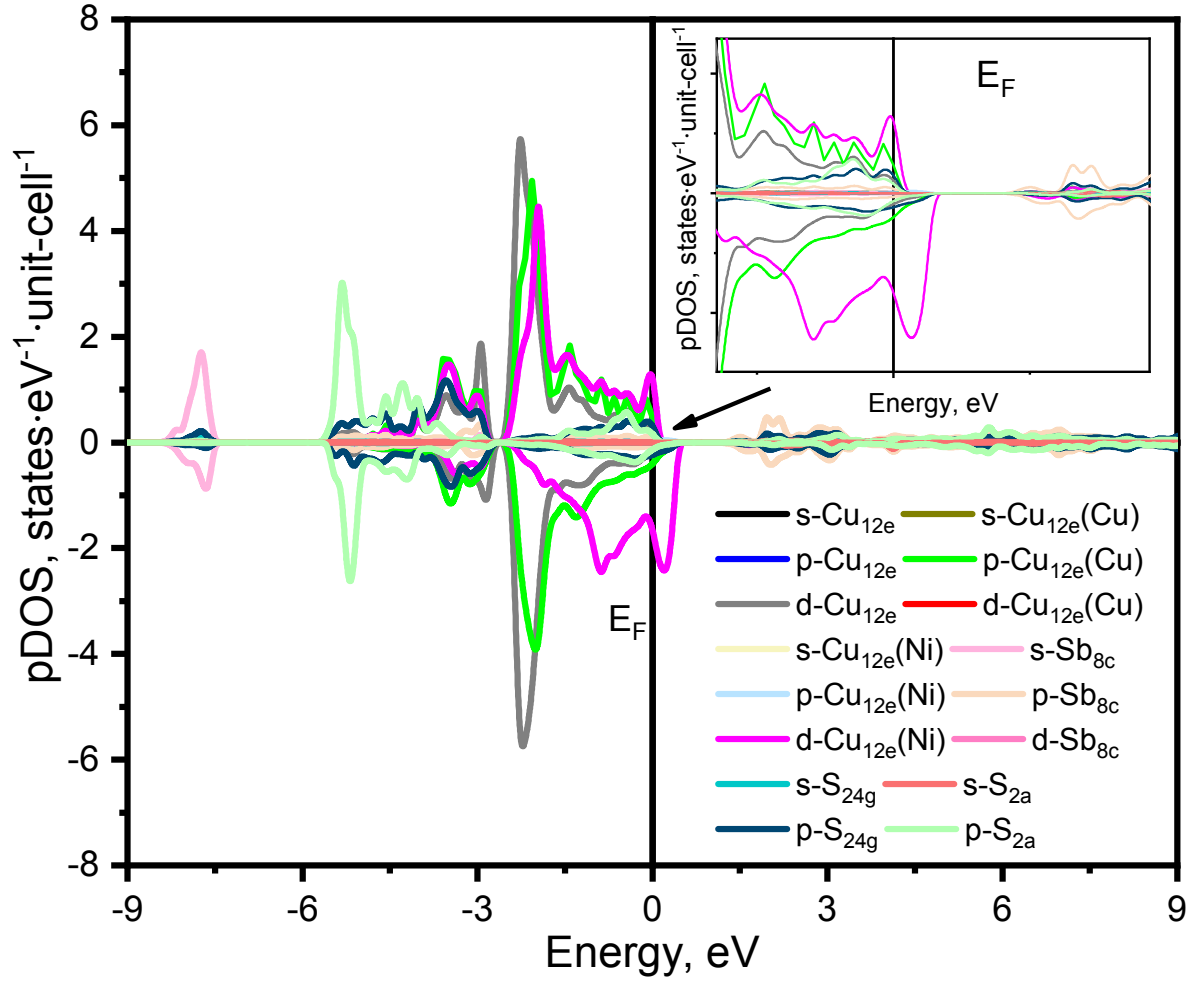


Fig. S9. Spin-polarized pDOS of $\text{Cu}_{11}\text{Ni}_1\text{Sb}_4\text{S}_{13}$ obtained from AkaiKKR-CPA calculations. Vertical line indicates the Fermi level (0 eV)