

Supplementary information for “Cobalt-Based Magnetic Weyl Semimetals with High-Thermodynamic Stabilities ”

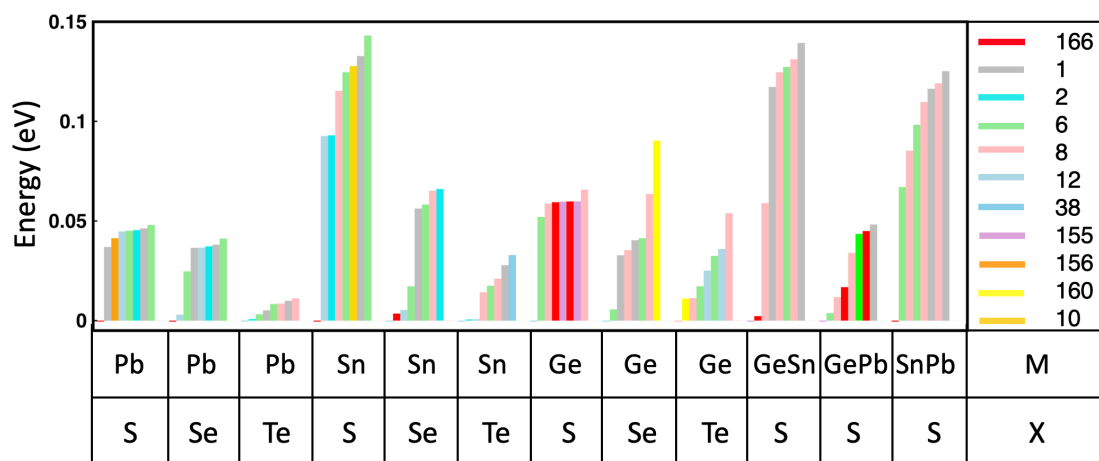
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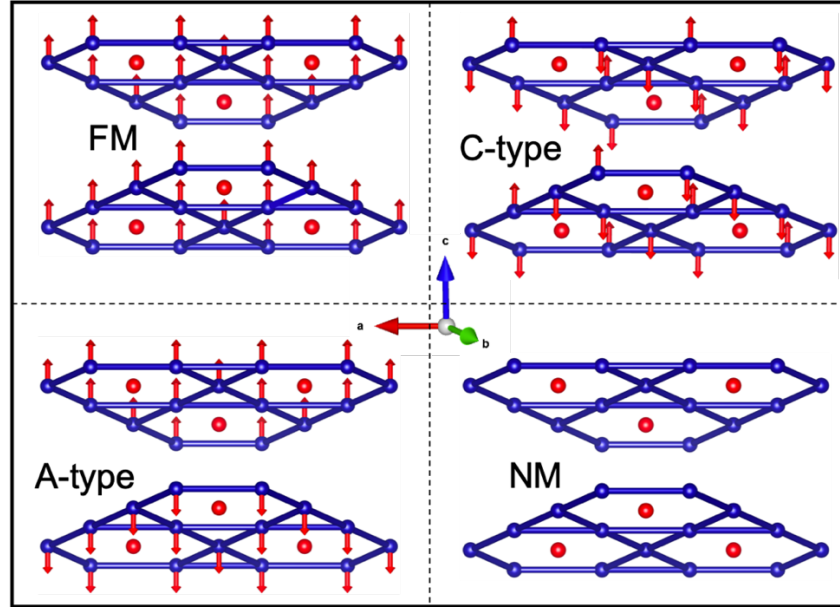
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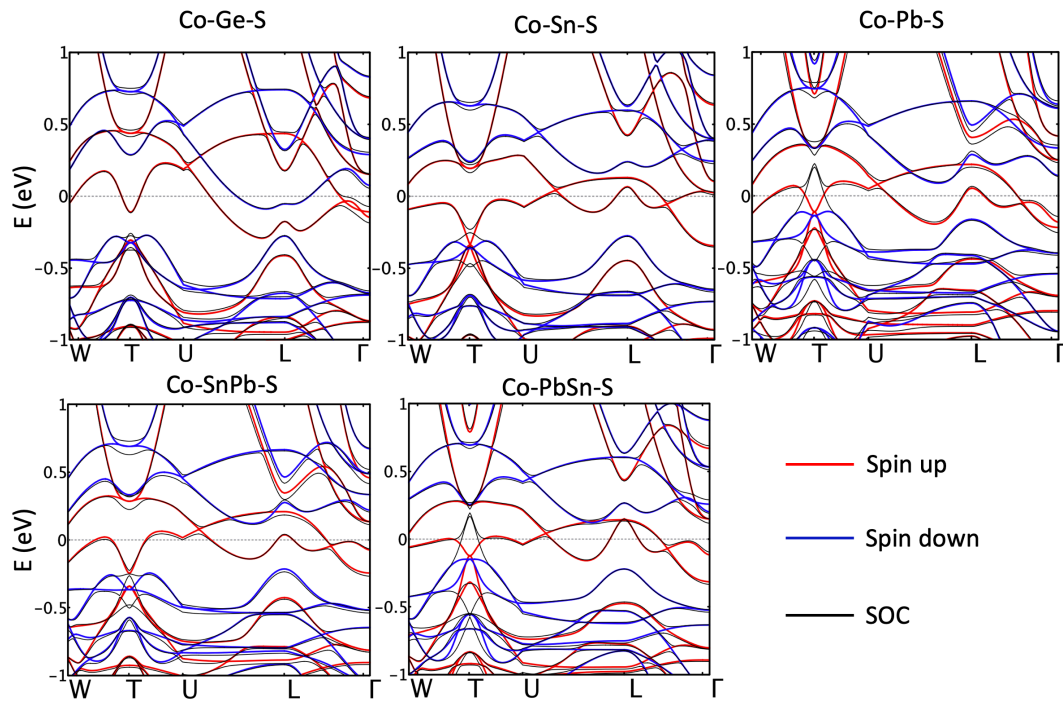
Supplementary Figures



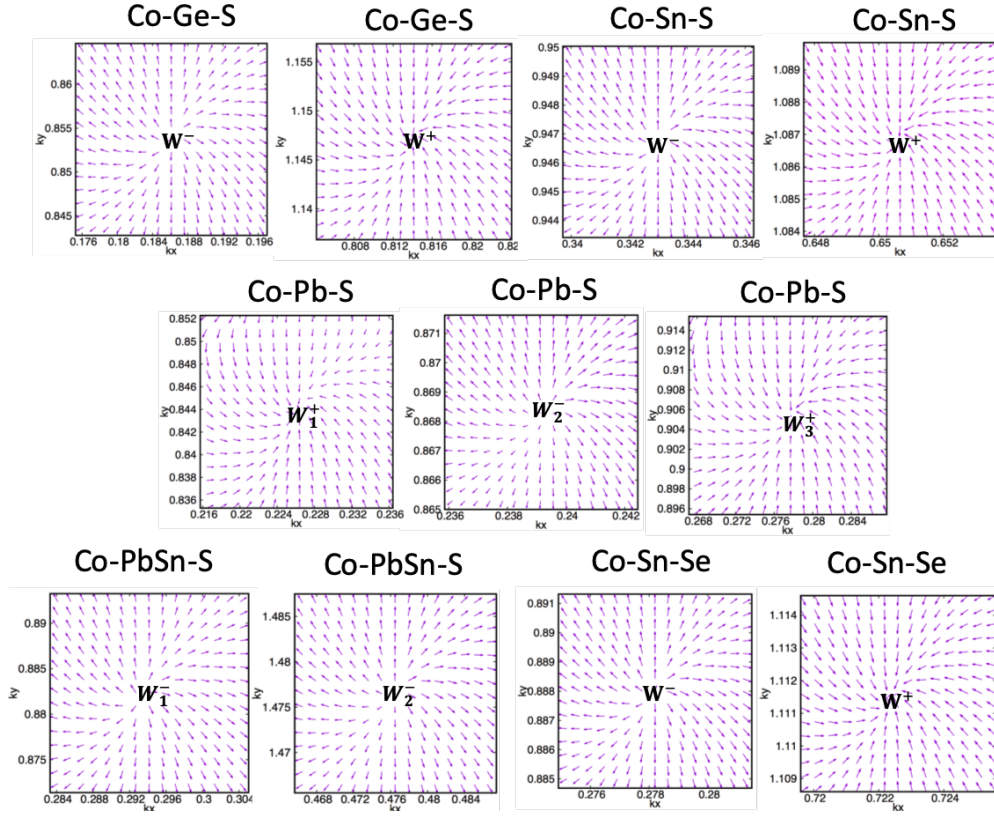
Supplementary Figure 1. The energy of the stable and metastable crystal phases of Co-MM'-X (M/M'=Ge, Sn, Pb and X=S, Se, Te) found by particle swarm optimization based on first-principles density functional theory calculations (see main text for details); here the energy is calculated with respect to the ground state structure of a given compound.



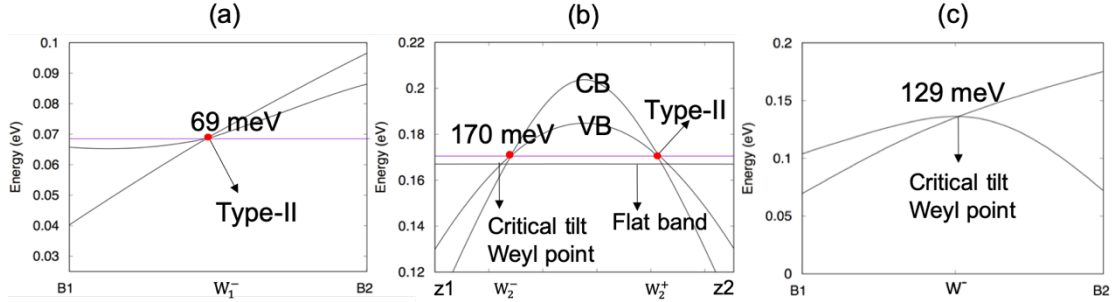
Supplementary Figure 2. Ferromagnetic (FM), antiferromagnetic (AFM, A-type and C-type phases), and nonmagnetic (NM) spin states of shandites. A-type AFM phase represents AFM spin configurations between the layers, while C-type AFM has intralayer AFM and interlayer FM spin configurations. The blue and red balls represent Co and metal atoms, respectively. The red arrow represents the spin orientation. For simplicity, we leave out X and M' atoms.



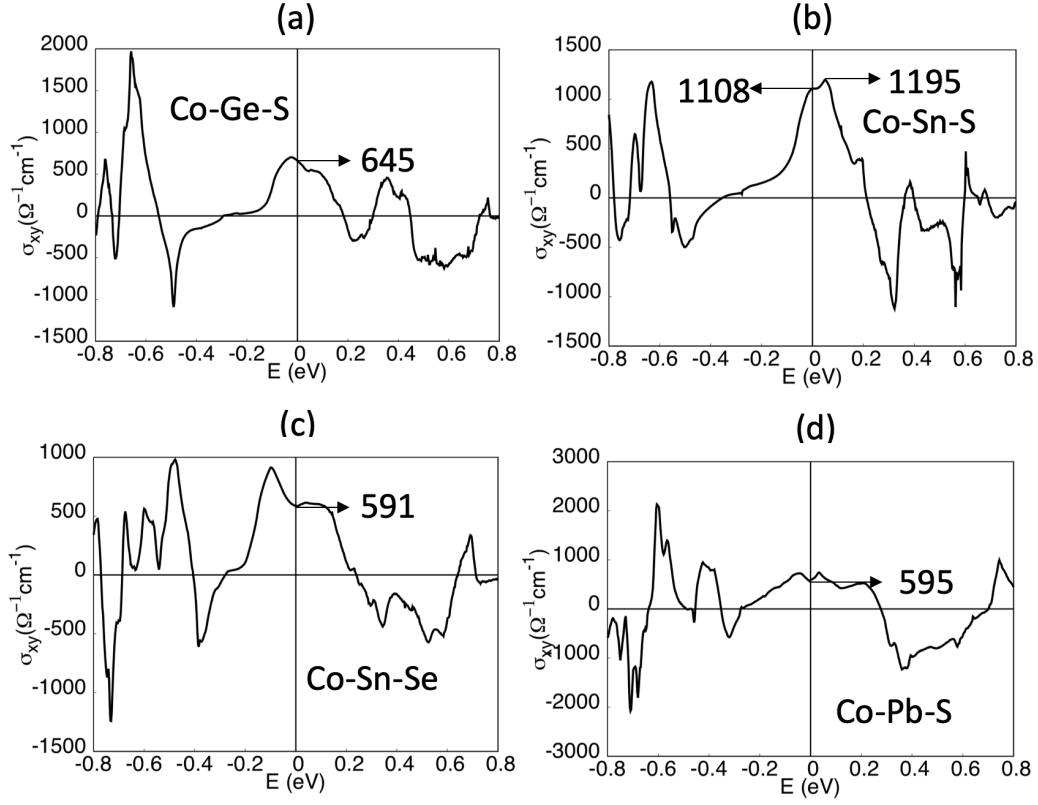
Supplementary Figure 3. Band structures of Co-MM'-S without/with SOC effects. Nodal lines of all the band structures are centered at the L point.



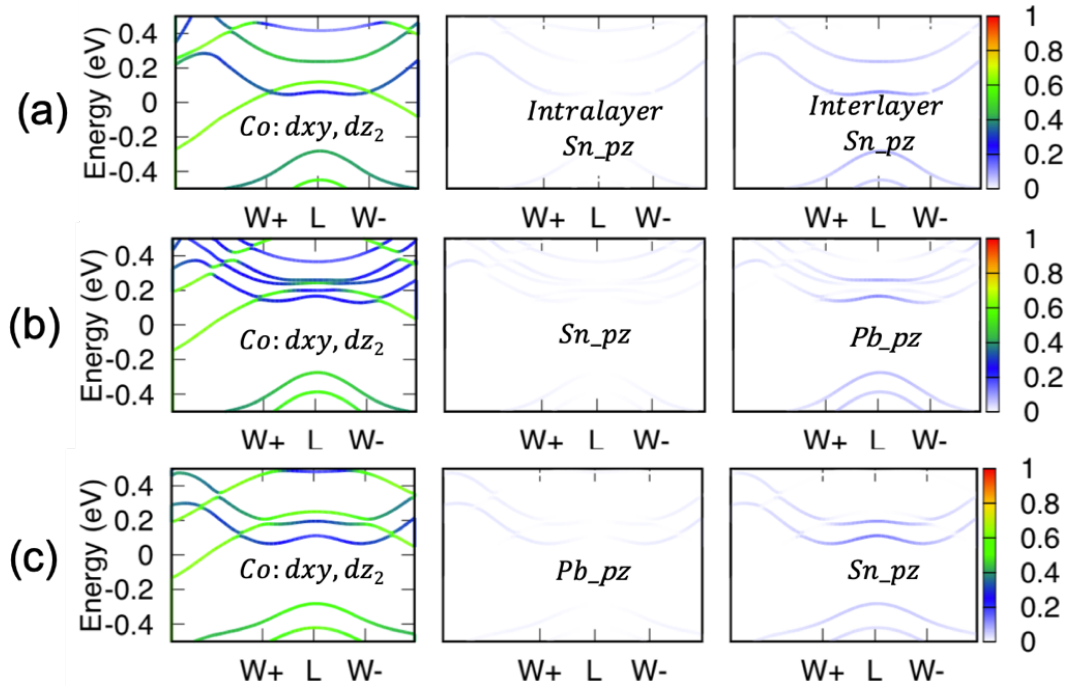
Supplementary Figure 4. Berry curvature around Weyl points for Co based Shandite structures. “+” and “-” represent the chirality of the Weyl point, i.e. the propagation of Weyl Fermion parallel and anti-parallel to their spin orientation



Supplementary Figure 5. (a) Band structure for Co-PbSn-S with a k path across the Weyl point (W_1^- , see main text). (b) Band structure for Co-PbSn-S with k path along the C_{3z} rotational axis (z axis in real space). The position of this pair of Weyl points can be found in the Table S2. CB and VB represent the conduction band and valence band. Under the VB band, one can see there exist a flat band pierce the VB and CB bands and form four critical Weyl points (c) Band structure for Co-Sn-Se with a k path across the Weyl point. One can see that the dispersion of the band crossing is critical tilt, i.e., locating at the boundary of type-I and type-II Weyl semimetal.

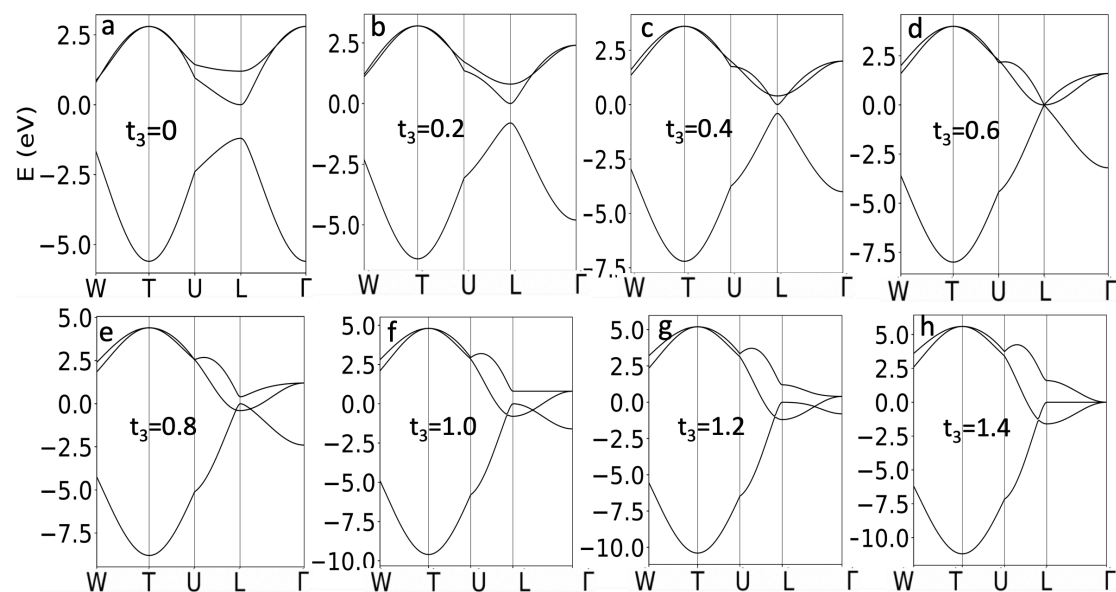


Supplementary Figure 6. AHC for Co-Ge-S (a), Co-Sn-S (b), Co-Sn-Se (c) and Co-Pb-S (d) systems.

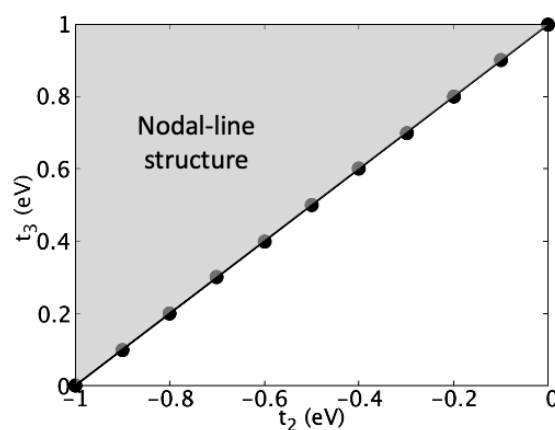


Supplementary Figure 7. Fat bands for CoSnS (a), CoSnPbS (b) and CoPbSnS (c). One can see that the band inversion is mainly contributed by the d_{xy} and d_{z^2} of Co

atoms. The intralayer M sites almost have no contribution for the band inversion bands, while the interlayer M' sites have much more contributions compared with that of intralayer M sites.



Supplementary Figure 8. TB band structures change with parameter t_3 . The $t_I = -1.0$ eV and $t_2 = -0.4$ eV are fixed. One can see that the NN interlayer coupling (t_3) between Co atoms cause the band inversion nodal line.



Supplementary Figure 9. The relation between t_2 and t_3 that delineates the boundary values to reproduce the nodal line for $t_I = -1.0$ eV. All the parameters in the grey region reproduce the nodal line structure. For example, for $t_2 = -0.8$ eV (-0.6 eV, -0.4 eV), the nodal line emerges when the $t_3 > 0.2$ eV (0.4 eV, 0.6 eV).

Supplementary Tables

Compounds	FM (eV)	C-AFM (eV)	A-AFM (eV)	NM (eV)	FM-NM (meV)
Co-Ge-S	-40.20201	(FM)	(NM)	-40.19843	-3.6
Co-Sn-S	-39.48557	(FM)	-39.46494	-39.46077	-24.8
Co-Pb-S	-37.88600	(FM)	-37.86313	-37.86350	-22.5
Co-Sn-Se	-37.21521	(FM)	(NM)	-37.19939	-15.8
Co-Pb-Se	-35.77054	(FM)	(NM)	-35.76505	-5.5
Co-GeSn-S	-39.83252	(FM)	(NM)	-39.82633	-6.0
Co-GePb-S	-38.92828	(FM)	(NM)	-38.92440	-3.9
Co-SnPb-S	-38.66832	(FM)	38.64778	-38.64717	-21.2
Co-PbSn-S	-38.62266	(FM)	(FM)	-38.59525	-27.4

Supplementary Table 1. The total energies for difference magnetic states. The C-AFM state will optimize to the FM state for all the compounds and A-AFM state will optimize to the NM state for Co-Ge-S, Co-Sn-Se, Co-Pb-Se, Co-GeSn-S, and Co-GePb-S.

Compounds	Weyl point	kx	ky	kz	Type	Chirality	E-E _F (meV)	K _b =K _c plane	Total number of Weyl points
Co-Ge-S	W ⁻	0.186	0.853	0.853	II	-1	134	Yes	2×3(C _{3z})=6
	W ⁺	0.814	1.147	1.147	II	+1	134	Yes	
Co-Sn-S	W ⁻	0.343	0.947	0.947	I	-1	58	Yes	2×3(C _{3z})=6
	W ⁺	0.657	1.053	1.053	I	+1	58	Yes	
Co-Sn-Se	W ⁻	0.278	0.888	0.888	critical	-1	129	Yes	2×3(C _{3z})=6
	W ⁺	0.722	1.112	1.112	critical	+1	129	Yes	
Co-Pb-S	W ₁ ⁺	0.226	0.844	0.844	II	+1	37	Yes	6×3(C _{3z})+4×3(C _{3z}) ×2(M ₀₁₀)=42
	W ₁ ⁻	0.774	1.156	1.156	II	-1	37	Yes	
	W ₂ ⁻	0.239	0.868	0.868	II	-1	51	Yes	
	W ₂ ⁺	0.761	1.132	1.132	II	+1	51	Yes	
	W ₃ ⁺	0.278	0.905	0.905	II	+1	82	Yes	
	W ₃ ⁻	0.722	1.095	1.095	II	-1	82	Yes	
	W ₄ ⁻	0.113	0.799	0.227	I	-1	5	No	
	W ₄ ⁺	-0.113	-0.799	-0.227	I	+1	5	No	
	W ₅ ⁺	-0.022	0.912	0.337	I	+1	88	No	
	W ₅ ⁻	0.022	-0.912	-0.337	I	-1	88	No	
Co-PbSn-S	W ₁ ⁻	0.294	0.882	0.882	II	-1	69	Yes	2×3(C _{3z}) +2(z axis)=8
	W ₁ ⁺	0.706	1.118	1.118	II	+1	69	Yes	
	W ₂ ⁻	0.476	1.476	1.476	II	-1	170	Yes	
	W ₂ ⁺	0.524	0.524	0.524	II	+1	170	Yes	

Supplementary Table 2. The position, type, chirality, energy level and number of Weyl point for Co-Ge-S, Co-Sn-S, Co-Sn-Se, Co-Pb-S and Co-PbSn-S shandite structures. The last column 3(C_{3z}) means the multiple 3 is caused by the C_{3z} symmetry. 2(M₀₁₀) means the multiple 2 is due to M₀₁₀ symmetry. 2(z axis) means the two Weyl points locate at the z axis, thus, it does not induce other Weyl points under C_{3z} and M₀₁₀ symmetry.

TRIM	Γ	L($\times 3$)	M($\times 3$)	Z	Product
CoSnPbS	+1	-1	-1	+1	+1

Supplementary Table 3: Parities (inversion eigenvalues) for the eight TRIM points (one Γ point, three L points and three M points) for Co-SnPb-S system which are calculated from the occupied bands. The product of the eigenvalues for eight TRIM points equal to positive 1.