Electronic Supplementary Material (ESI) for Materials Advances.

Supplementary Materials

High-throughput screening of stable sulfide semiconductors for solar cell conversion

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Supplementary Figures

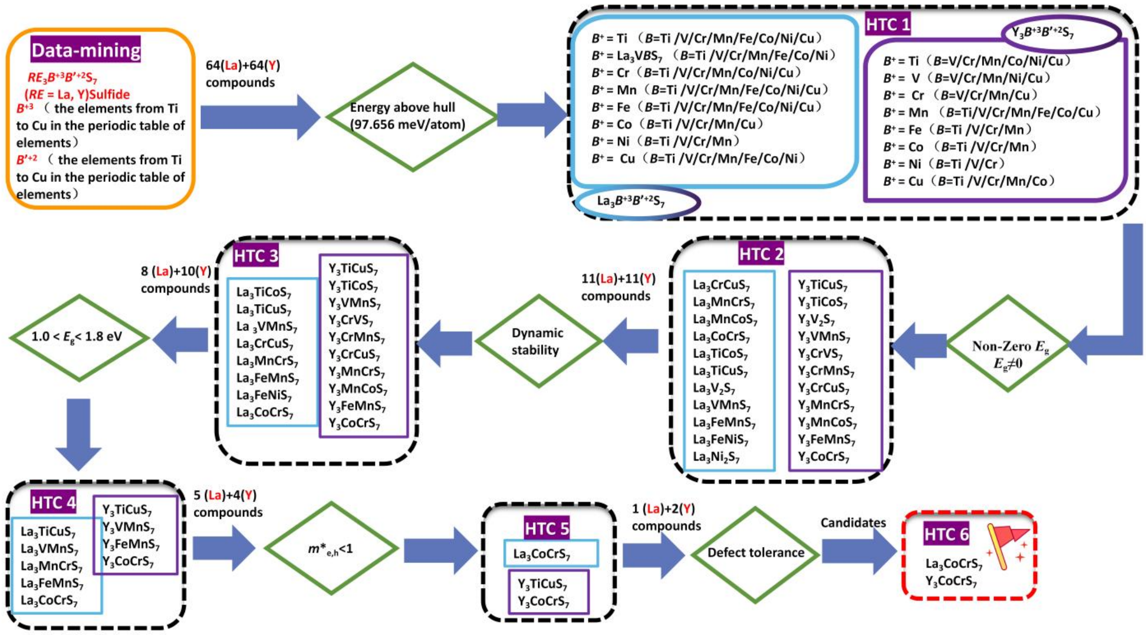
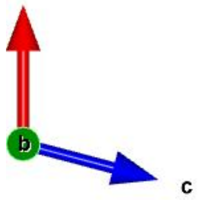
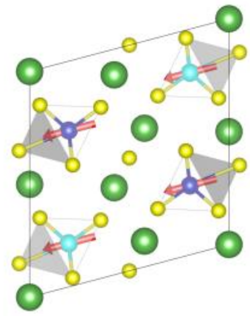
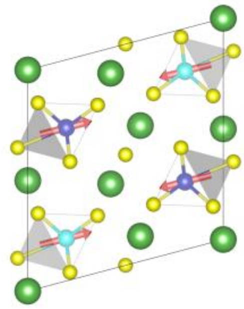
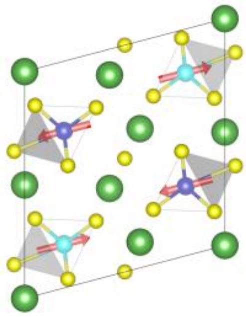
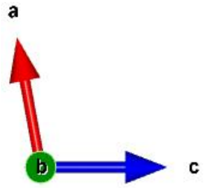
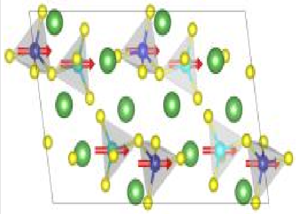
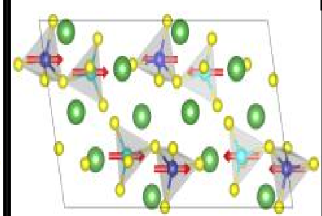
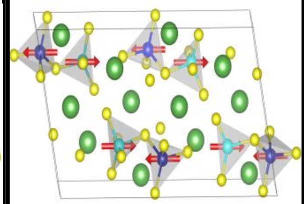
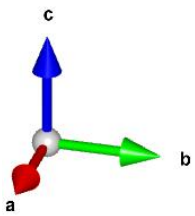
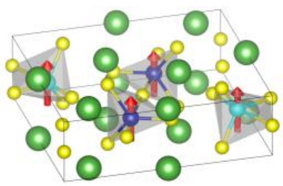
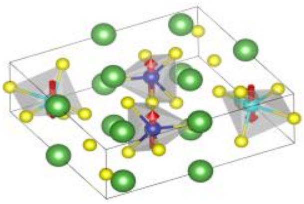
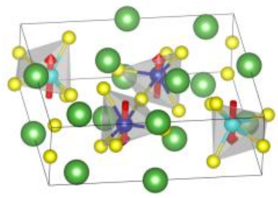
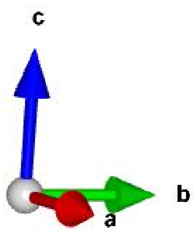
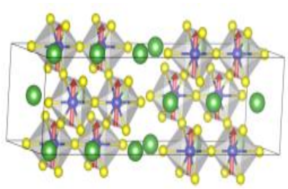
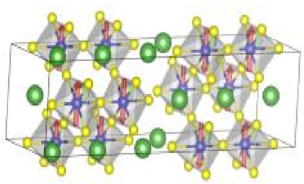
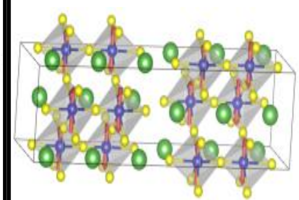


Fig. S1 The workflows of HTC. Schematic representation of the screening process for $RE_3BB'S_7$ (*RE* = La, Y; *B*/*B*' = Ti - Cu) compounds with detailed DFT analysis.

Space Group	FM	AFM1	AFM2
C*2/*m 			
P*2$_1$/*c 			
Pbam 			
Cccm 			

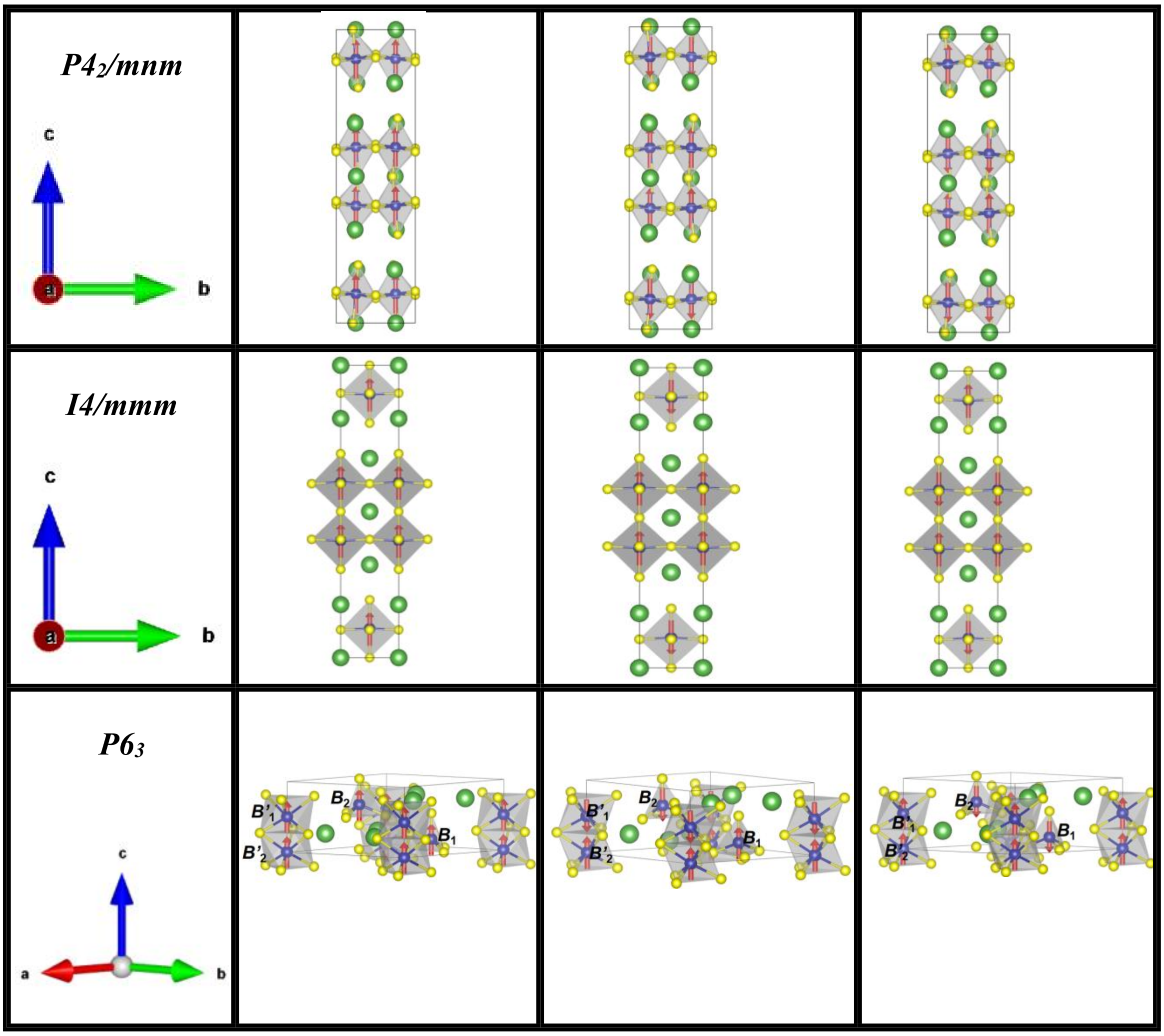


Fig. S2 Scheme for different magnetic structures in $A_3B_2S_7$. The green, blue and yellow spheres represent the *A*, *B* and sulfur atoms respectively. The spin moment is along [001] (out-of plane) direction and arrows represent the magnetic moment direction.

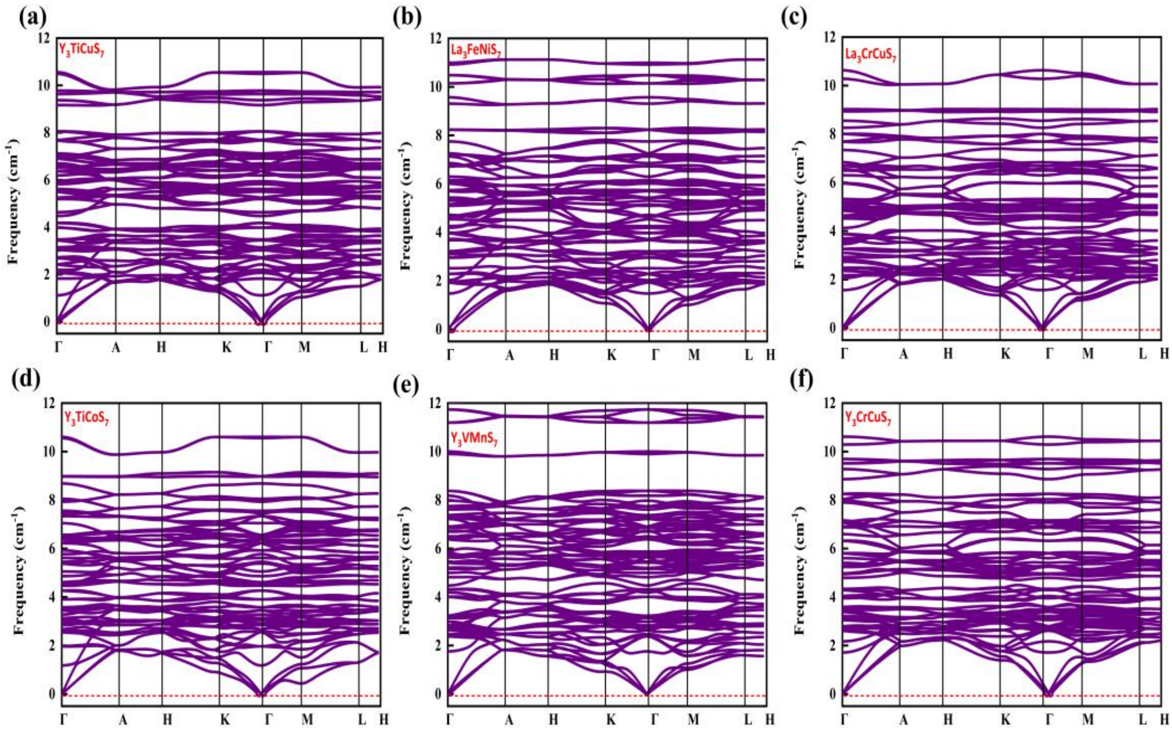


Fig. S3 Partial phonon dispersion of selected stable partial $A_3BB'S_7$ sulfides.

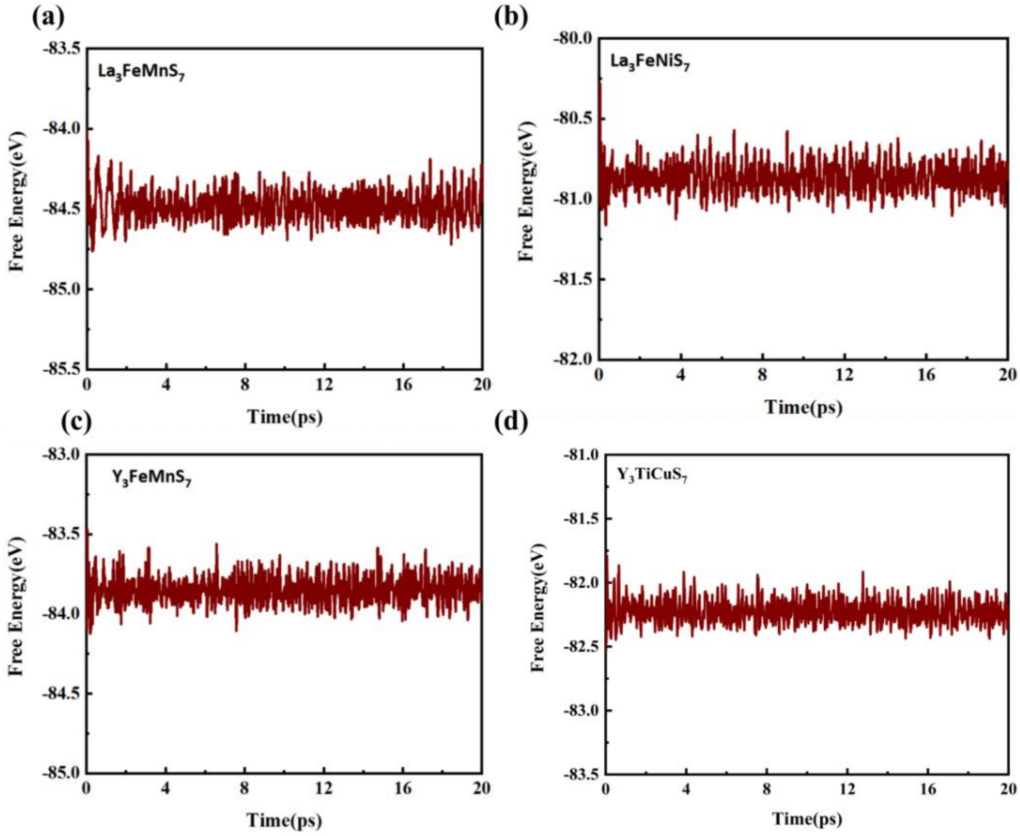


Fig. S4 Variations of the total potential energy of partial stable $A_3BB'S_7$ sulfides with respect to simulation time during ab initio molecular dynamics simulations.

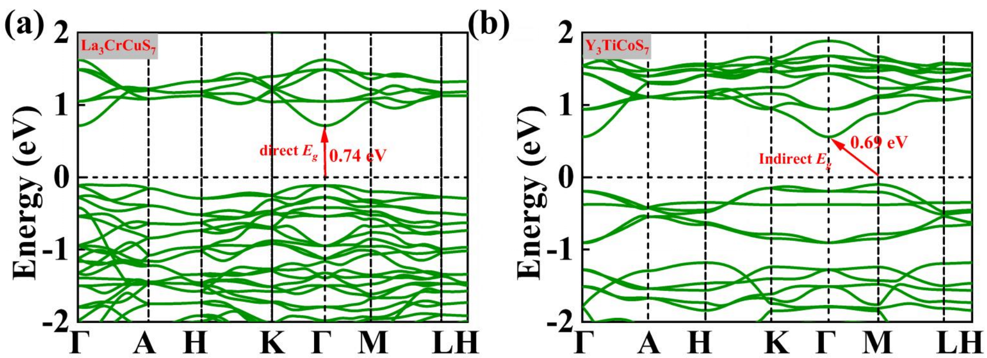


Fig. S5 Band structure of partial stable $A_3BB'S_7$ sulfides. The upward arrow represents direct or indirect E_g.

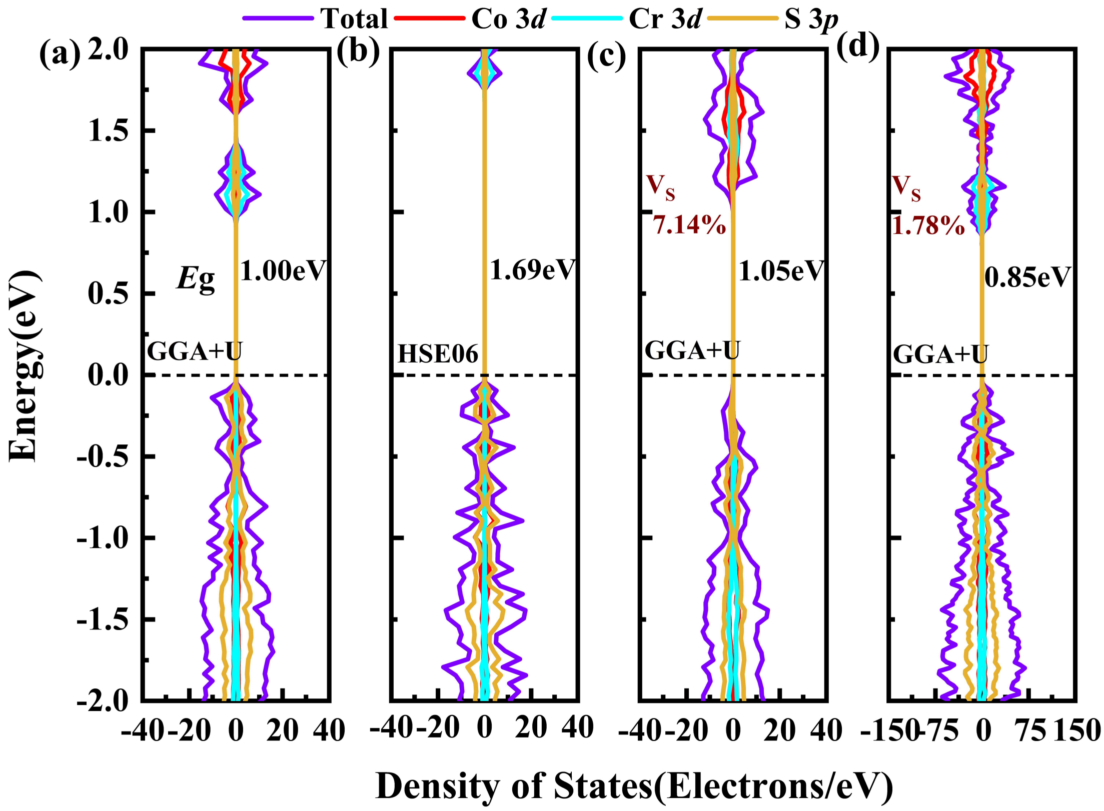


Fig. S6 The electronic structures of Y_3CoCrS_7. Total DOSs for pristine Y_3CoCrS_7 from (a) GGA+U and (b) HSE06 methods. Total DOSs for Y_3CoCrS_7 with S vacancy concentration (c) 7.14% and (d) 1.78% from GGA+U method. No additional bands are produced. The zero of the energy is set at the Fermi level.

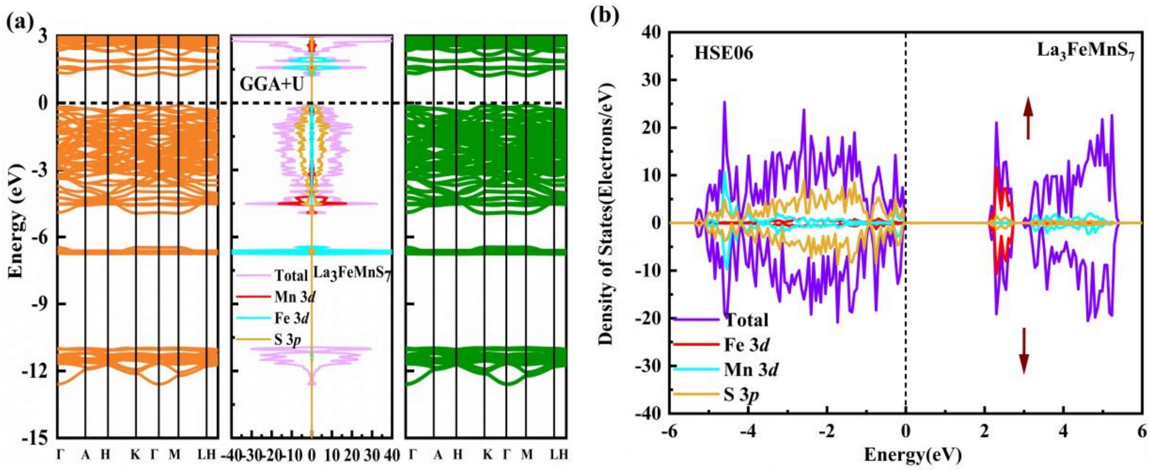


Fig. S7 The electronic structures of La_3FeMnS_7. Total DOSs and band structure from (a) GGA+U and (b) HSE06 methods. Band structure including down-spin band (left), DOSs (middle) and up-spin band (right). The upward arrow represents the spin up, and the downward arrow means the spin down.

Supplementary Tables

Table S1 The corresponding lattice parameters, tolerance factors(τ) and properties of the representative compounds with seven kinds of crystal structures in the $A_3B_2S_7$ system. The Goldschmidt tolerance factor, which is used as a simple measure to predict tendency towards octahedral rotations, and is originally defined in terms of the ionic radii r using $\tau = (r_A+r_S)/\sqrt{2}(r_B+r_S)$.

No.	Space Group	Existing Compound	Tolerance Factor (τ)	Properties	Refs.
1	*C*2/*m*	$Dy_3Sc_2S_7$	0.8183		1
		$Er_3Sc_2S_7$	0.8197		1
		$Gd_3Sc_2S_7$	0.8348		1
		$Ho_3Sc_2S_7$	0.8238		1
		$Tb_3Sc_2S_7$	0.8293		1
2	$P2_1/c$	$Ba_3Sn_2S_7$	0.9520		2
3	*Pbam*	$Eu_3Sn_2S_7$	0.9077		3
4	*Cccm*	$Ba_3Zr_2S_7$	0.9479		4
5	$P4_2/mnm$	$Ba_3Zr_2S_7$	0.9479	E_g = 1.28 eV	5
6	*I*4/*mmm*	$Ba_3Zr_2S_7$	0.9479		6
7	$P6_3$	$La_3Co_2S_7$	0.9803		7

		La_3FeMnS_7		*p*-type semiconductor	8
		$La_3Fe_2S_7$	0.9277	*p*-type semiconductor	8,9
		La_3FeCoS_7	0.9533	*p*-type semiconductor	8
		La_3FeNiS_7	0.9492		8
		La_3FeMgS_7		*p*-type semiconductor	8
		La_3FeZnS_7		*p*-type semiconductor	8
		La_3MnAlS_7		AFM	8
		La_3FeAlS_7		AFM	8
		La_3CoAlS_7		AFM	8
		La_3AgGeS_7			10
		La_3CuGeS_7			11,12

		La_3CuSnS_7			13
		La_3AgSiS_7			14
		La_3AgSnS_7			15
		La_3FeGaS_7			16
		La_3CoGaS_7			16
		La_3CuGaS_7			17
		La_3FeInS_7		AFM $T_N = 30$ K	18
		La_3CoInS_7			18
		La_3NiInS_7			18
		$U_3Cu_2S_7$		Paramagnetism (PM)	19
		Y_3CuSnS_7			20
		Y_3CuSiS_7			12,21
		Y_3CoGaS_7			
		Y_3CuGeS_7			22
		Y_3NaSiS_7			23
		Ce_3CuGeS_7			24
		Pr_3CuGeS_7			24
		Nd_3CuGeS_7			24

		Sm_3CuGeS_7			24,25
		Gd_3CuGeS_7			24
		Tb_3CuGeS_7			24
		Dy_3CuGeS_7			12,24
		Er_3CuGeS_7			24
		Ho_3CuGeS_7			26
		Ce_3CuSnS_7			13
		Pr_3CuSnS_7			13
		Nd_3CuSnS_7			13
		Sm_3CuSnS_7			13
		Gd_3CuSnS_7			13
		Tb_3CuSnS_7			13
		Dy_3CuSnS_7			13
		Er_3CuSnS_7			13
		Ce_3CuSiS_7			27,28
		Pr_3CuSiS_7			27
		Nd_3CuSiS_7			27
		Sm_3CuSiS_7			27
		Gd_3CuSiS_7			27,29
		Tb_3CuSiS_7			27

		Dy_3CuSiS_7			27
		Er_3CuSiS_7			27
		Ho_3CuSiS_7			12,26
		Ce_3FeGaS_7			16
		Pr_3FeGaS_7		PM	16
		Nd_3FeGaS_7		PM	16
		Tb_3FeGeS_7		AFM T_N = 15 K	16
		Sm_3FeGeS_7			16
		Gd_3FeGeS_7		PM	16
		Ce_3CoGaS_7			16
		Pr_3CoGaS_7		AFM T_N < 2 K	16
		Nd_3CoGaS_7		PM	16
		Tb_3CoGeS_7		AFM T_N =3 K	16
		Sm_3CoGeS_7			16
		Gd_3CoGeS_7		PM	16
		Dy_3CoGaS_7		AFM T_N = 2 K	16
		Ho_3CoGaS_7		PM	16
		Er_3CoGaS_7		AFM T_N=3 K	16
		Ce_3NiGaS_7		PM	16
		Tb_3NiGaS_7		PM	16

		Ce_3CuGaS_7			17
		Pr_3CuGaS_7			17
		Nd_3CuGaS_7			17
		Yb_3NaGeS_7			30
		Sm_3NaGeS_7			30
		Nd_3NaGeS_7			30
		Gd_3NaGeS_7			30
		Ce_3NaGeS_7			30
		Ce_3AgGeS_7			12
		Pr_3AgGeS_7			12

Table S2 Structural optimization energy (eV) of $La_3B_2S_7$ (B =Ti - Cu). The lowest energy of each compound is in red. "-" represents the case of non-convergence, and the corresponding magnetic structure is abandoned.

		C2/m	*P2₁/c*	*Pbam*	*Cccm*	*P4₂/mnm*	*I4/mmm*	*P6₃*
$La_3Ti_2S_7$	FM	-79.0028	-80.9655	-81.5642	-80.5690	-81.1527	-80.5422	-81.4493
	AFM1	-78.8786	-80.9652	-81.5824	-80.5693	-81.1529	-80.5422	-81.3941
	AFM2	-78.8796	-	-81.5059	-80.5692	-81.1522	-80.5418	-81.4167
$La_3V_2S_7$	FM	-79.1007	-81.1459	-81.8160	-80.7491	-81.5608	-80.7382	-81.9907
	AFM1	-79.1046	-81.0816	-81.7866	-80.7756	-81.5597	-80.7670	-82.0120
	AFM2	-79.0845	-81.1412	-81.8428	-80.7868	-81.5718	-80.7677	-82.1145
$La_3Cr_2S_7$	FM	-79.0537	-81.2477	-82.0815	-81.1372	-81.8166	-81.1286	-81.5264
	AFM1	-79.0869	-81.2465	-82.0779	-81.1442	-81.8180	-81.1266	-81.5490
	AFM2	-79.0886	-81.2300	-82.1480	-81.1445	-81.7880	-81.1254	-81.6253
$La_3Mn_2S_7$	FM	-78.1689	-80.6067	-81.1291	-79.9878	-80.5212	-79.9991	-80.8442
	AFM1	-78.2732	-78.3865	-81.1561	-79.8404	-80.5285	-79.9965	-80.8225
	AFM2	-78.2686	-	-80.9106	-79.8493	-80.5255	-79.8474	-80.8491
$La_3Fe_2S_7$	FM	-75.0625	-76.7535	-78.0753	-77.2203	-77.4800	-77.2263	-78.2612
	AFM1	-75.1299	-76.7459	-78.1250	-77.1592	-77.4828	-77.2347	-78.2729
	AFM2	-	-76.7509	-77.9881	-77.1704	-77.4794	-77.1835	-78.2733
$La_3Co_2S_7$	FM	-71.6212	-74.4072	-74.9871	-74.6749	-74.6610	-74.6956	-75.1126
	AFM1	-71.7118	-74.5405	-74.9742	-74.6737	-74.6599	-74.6964	-75.1125
	AFM2	-71.7111	-74.4573	-74.9752	-74.6752	-74.6613	-74.6960	-75.1212
$La_3Ni_2S_7$	FM	-68.9322	-71.7056	-72.4252	-72.2185	-72.2832	-72.2832	-71.9069
	AFM1	-68.9328	-71.7035	-72.4252	-72.2185	-72.2816	-72.2816	-71.9783
	AFM2	-	-71.7045	-72.4259	-72.2185	-72.2821	-72.2821	-72.0952
$La_3Cu_2S_7$	FM	-65.0876	-67.8474	-68.3434	-67.6337	-67.8139	-67.6447	-67.7898
	AFM1	-65.0713	-67.8423	-68.3452	-67.6321	-67.8134	-67.6447	-67.7908
	AFM2	-	-67.8384	-68.3437	-67.6392	-67.8125	-67.6453	-67.7908

Table S3 Thermodynamic screening details of $La_3BB'S_7$ (B/B' = Ti-Cu) by E_{hull}(meV/atom). The material project IDs (mp-number) of the compounds on the convex hull are marked in the parentheses.

Compounds	**Space group**	**Magnetic ground state**	**Compounds on the convex hull**	E_{hull} **(meV/atom)**
La_3TiTiS_7	*Pbam*	AFM1	La_2S_3 (mp-7475)+ Ti_2S_3(mp-1101099) + TiS(mp-1018028)	72.4041
La_3TiVS_7	$P6_3$	AFM2	La_2S_3 + Ti_2S_3 + VS(mp-1868)	52.4691
La_3TiCrS_7	$P6_3$	AFM2	La_2S_3 + Ti_2S_3 + CrS(mp-523)	53.2071
La_3TiMnS_7	$P6_3$	AFM2	La_2S_3 + Ti_2S_3 + MnS(mp-2065)	36.1407
La_3TiFeS_7	$P6_3$	AFM1	La_2S_3 + Ti_2S_3 + FeS(mp-505531)	75.5514
La_3TiCoS_7	$P6_3$	AFM2	La_2S_3 + Ti_2S_3 + CoS(mp-1147746)	56.2159
La_3TiNiS_7	$P6_3$	AFM1	La_2S_3 + Ti_2S_3 + NiS(mp-1547)	22.5923
La_3TiCuS_7	$P6_3$	AFM2	La_2S_3 + Ti_2S_3 + CuS(mp-555599)	-53.8920
La_3VTiS_7	$P6_3$	FM	La_2S_3 + V_3S_4(mp-799) + VS_2 (mp-1013525)+ TiS	79.6366
La_3VVS_7	$P6_3$	AFM2	La_2S_3 + V_3S_4+ VS_2 + VS	39.0360
La_3VCrS_7	$P6_3$	AFM1	La_2S_3 + V_3S_4 + VS_2 + CrS	44.3347
La3$VMnS_7$	$P6_3$	AFM2	La_2S_3 + V_3S_4 + VS_2 + MnS	23.7688

La3VFeS_7	*P*6_3	AFM2	La_2S_3 + V_3S_4 + VS_2 + FeS	99.8159
La_3VCoS_7	*P*6_3	AFM1	La_2S_3 + V_3S_4 + VS_2 + CoS	83.3718
La_3VNiS_7	*P*6_3	AFM2	La_2S_3 + V_3S_4 + VS_2 + NiS	50.4504
La_3VCuS_7	*P*6_3	AFM1	La_2S_3 + V_3S_4 + VS_2 + CuS	-13.8973
La_3CrTiS_7	*P*6_3	AFM2	La_2S_3 + Cr_2S_3 + TiS	84.9772
La_3CrVS_7	*P*6_3	AFM2	La_2S_3 + Cr_2S_3 + VS	52.6952
La_3CrCrS_7	*Pbam*	AFM2	La_2S_3 + Cr_2S_3(mp-555569) + CrS	1.9465
La_3CrMnS_7	*P*6_3	FM	La_2S_3 + Cr_2S_3 + MnS	55.0713
La_3CrFeS_7	*P*6_3	AFM2	La_2S_3 + Cr_2S_3 + FeS	114.0645
La_3CrCoS_7	*P*6_3	FM	La_2S_3 + Cr_2S_3 + CoS	95.1014
La_3CrNiS_7	*P*6_3	AFM1	La_2S_3 + Cr_2S_3 + NiS	67.5784
La_3CrCuS_7	*P*6_3	FM	La_2S_3 + Cr_2S_3 + CuS	-4.8341
La_3MnTiS_7	*P*6_3	AFM2	La_2S_3 + Mn_2S_3(mp-974355) + TiS	-4.1385
La_3MnVS_7	*P*6_3	FM	La_2S_3 + Mn_2S_3 + VS	-11.5494
La_3MnCrS_7	*P*6_3	AFM2	La_2S_3 + Mn_2S_3 + CrS	-49.6299
La_3MnMnS_7	*Pbam*	AFM1	La_2S_3 + Mn_2S_3 + MnS	-25.2089
La_3MnFeS_7	*P*6_3	AFM2	La_2S_3 + Mn_2S_3 + FeS	71.5976
La_3MnCoS_7	*P*6_3	AFM2	La_2S_3 + Mn_2S_3 + CoS	50.7170
La_3MnNiS_7	*P*6_3	AFM1	La_2S_3 + Mn_2S_3 + NiS	62.4652

La_3MnCuS_7	$P6_3$	AFM1	$La_2S_3 + Mn_2S_3 + CuS$	4.7039
La_3FeTiS_7	$P6_3$	FM	$La_2S_3 + FeS_2 + FeS + TiS$	46.5559
La_3FeVS_7	$P6_3$	AFM2	$La_2S_3 + FeS_2 + FeS + VS$	23.6156
La_3FeCrS_7	$P6_3$	AFM2	$La_2S_3 + FeS_2 + FeS + CrS$	11.1703
La_3FeMnS_7	$P6_3$	AFM2	$La_2S_3 + FeS_2 + FeS + MnS$	13.2033
La_3FeFeS_7	$P6_3$	AFM2	$La_2S_3 + FeS_2$ (mp-1522)+ FeS	97.6561
La_3FeCoS_7	$P6_3$	AFM1	$La_2S_3 + FeS_2 + FeS + CoS$	95.6875
La_3FeNiS_7	$P6_3$	AFM2	$La_2S_3 + FeS_2 + FeS + NiS$	71.2535
La_3FeCuS_7	$P6_3$	AFM1	$La_2S_3 + FeS_2 + FeS + CuS$	70.7724
La_3CoTiS_7	$P6_3$	AFM1	La_2S_3 + Co_2S_3(mp-1183728) + TiS	38.4629
La_3CoVS_7	$P6_3$	AFM1	$La_2S_3 + Co_2S_3 + VS$	33.2514
La_3CoCrS_7	$P6_3$	AFM2	$La_2S_3 + Co_2S_3 + CrS$	-2.1264
La_3CoMnS_7	$P6_3$	AFM2	$La_2S_3 + Co_2S_3 + MnS$	44.4441
La_3CoFeS_7	$P6_3$	FM	$La_2S_3 + Co_2S_3 + FeS$	109.7625
La_3CoCoS_7	$P6_3$	AFM2	$La_2S_3 + Co_2S_3 + CoS$	98.0343
La_3CoNiS_7	$P6_3$	AFM2	$La_2S_3 + Co_2S_3 + NiS$	106.1718
La_3CoCuS_7	$P6_3$	AFM2	$La_2S_3 + Co_2S_3 + CuS$	86.2314
La_3NiTiS_7	$P6_3$	AFM1	La_2S_3 + Ni_3S_4(mp-1050) + NiS_2 (mp-1180046)+	38.7534

			TiS	
La_3NiVS_7	*P*6_3	AFM1	$La_2S_3 + Ni_3S_4 + NiS_2 + VS$	38.4501
La_3NiCrS_7	*P*6_3	AFM2	$La_2S_3 + Ni_3S_4 + NiS_2 + CrS$	11.4520
La_3NiMnS_7	*P*6_3	AFM2	$La_2S_3 + Ni_3S_4 + NiS_2 + MnS$	45.0506
La_3NiFeS_7	*P*6_3	FM	$La_2S_3 + Ni_3S_4 + NiS_2 + NiS$	113.4404
La_3NiCoS_7	*P*6_3	FM	$La_2S_3 + Ni_3S_4 + NiS_2 + CoS$	105.3345
La_3NiNiS_7	*Pbam*	AFM2	$La_2S_3 + Ni_3S_4 + NiS_2 + NiS$	75.7763
La_3NiCuS_7	*P*6_3	AFM2	$La_2S_3 + Ni_3S_4 + NiS_2 + CuS$	114.4140
La_3CuTiS_7	*P*6_3	AFM2	La_2S_3 + $LaCuS_2$(mp-4841) + CuS_2 + TiS	-15.4209
La_3CuVS_7	*P*6_3	AFM1	$La_2S_3 + CuS_2 + LaCuS_2 + VS$	4.2010
La_3CuCrS_7	*P*6_3	AFM2	$La_2S_3 + CuS_2 + LaCuS_2 + CrS$	-29.7537
La_3CuMnS_7	*P*6_3	AFM2	$La_2S_3 + CuS_2 + LaCuS_2 + MnS$	14.6570
La_3CuFeS_7	*P*6_3	AFM1	$La_2S_3 + CuS_2 + LaCuS_2 + FeS$	81.4995
La_3CuCoS_7	*P*6_3	FM	$La_2S_3 + CuS_2 + LaCuS_2 + CoS$	69.3299
La_3CuNiS_7	*P*6_3	AFM1	$La_2S_3 + CuS_2 + LaCuS_2 + NiS$	93.3187
La_3CuCuS_7	*Pbam*	AFM1	$La_2S_3 + CuS_2 + LaCuS_2 + CuS$	65.1781

Table S4 Thermodynamic screening details of $Y_3BB'S_7$ (B/B' = Ti-Cu) by E_{hull} (meV/atom). The material project IDs (mp-number) of the compounds on the convex hull are marked in the parentheses.

Compounds	Space group of the lowest energy	Magnetic Ground state	Compounds on the convex hull	E_{hull} (meV/atom)
Y_3TiTiS_7	$P6_3$	AFM1	Y_2S_3 (mp-541289)+ Ti_2S_3 + TiS	127.1136
Y_3TiVS_7	$P6_3$	AFM2	Y_2S_3 + Ti_2S_3 + VS	92.6394
Y_3TiCrS_7	$P6_3$	AFM2	Y_2S_3 + Ti_2S_3 + CrS	94.2864
Y_3TiMnS_7	$P6_3$	AFM2	Y_2S_3 + Ti_2S_3 + MnS	79.0006
Y_3TiFeS_7	$P6_3$	AFM2	Y_2S_3 + Ti_2S_3 + FeS	117.7677
Y_3TiCoS_7	$P6_3$	AFM2	Y_2S_3 + Ti_2S_3 + CoS	95.5547
Y_3TiNiS_7	$P6_3$	AFM1	Y_2S_3 + Ti_2S_3 + NiS	78.9549
Y_3TiCuS_7	$P6_3$	FM	Y_2S_3 + Ti_2S_3 + CuS	5.7233
Y_3VTiS_7	$P6_3$	AFM1	Y_2S_3 + V_3S_4(mp-799) + VS_2 + TiS	120.1466
Y_3VVS_7	$P6_3$	AFM2	Y_2S_3 + V_3S_4 + VS_2 + VS	76.7273
Y_3VCrS_7	$P6_3$	AFM2	Y_2S_3 + V_3S_4 + VS_2 +CrS	84.5787
Y_3VMnS_7	$P6_3$	AFM2	Y_2S_3 + V_3S_4 + VS_2 +MnS	68.2859
Y_3VFeS_7	$P6_3$	AFM1	Y_2S_3 + V_3S_4 + VS_2 + FeS	139.5178
Y_3VCoS_7	$P6_3$	FM	Y_2S_3 + V_3S_4 + VS_2 + CoS	124.4004

Y_3VNiS_7	*P*6_3	AFM1	$Y_2S_3 + V_3S_4 + VS_2 + NiS$	95.3705
Y_3VCuS_7	*P*6_3	FM	$Y_2S_3 + V_3S_4 + VS_2 + CuS$	46.0255
Y_3CrTiS_7	*P*6_3	AFM1	$Y_2S_3 + Cr_2S_3 + TiS$	118.7115
Y_3CrVS_7	*P*6_3	AFM2	$Y_2S_3 + Cr_2S_3 +VS$	82.5292
Y_3CrCrS_7	*Pbam*	AFM1	$Y_2S_3 + Cr_2S_3 + CrS$	70.9144
Y_3CrMnS_7	*P*6_3	AFM2	$Y_2S_3 + Cr_2S_3 +MnS$	72.4296
Y_3CrFeS_7	*P*6_3	AFM1	$Y_2S_3 + Cr_2S_3 +FeS$	143.5902
Y_3CrCoS_7	*P*6_3	FM	$Y_2S_3 + Cr_2S_3 + CoS$	130.8638
Y_3CrNiS_7	*P*6_3	FM	$Y_2S_3 + Cr_2S_3 + NiS$	120.6573
Y_3CrCuS_7	*P*6_3	FM	$Y_2S_3 + Cr_2S_3 + CuS$	50.8652
Y_3MnTiS_7	*P*6_3	AFM1	$Y_2S_3 + Mn_2S_3 + TiS$	-8.7743
Y_3MnVS_7	*P*6_3	FM	$Y_2S_3 + Mn_2S_3 + VS$	26.4943
Y_3MnCrS_7	*P*6_3	AFM2	$Y_2S_3 + Mn_2S_3 + CrS$	-11.3827
Y_3MnMnS_7	*P*6_3	AFM2	$Y_2S_3 + Mn_2S_3 + MnS$	36.2013
Y_3MnFeS_7	*P*6_3	AFM1	$Y_2S_3 + Mn_2S_3 + FeS$	94.3493
Y_3MnCoS_7	*P*6_3	AFM2	$Y_2S_3 + Mn_2S_3 + CoS$	82.3617
Y_3MnNiS_7	*P*6_3	FM	$Y_2S_3 + Mn_2S_3 + NiS$	100.9952
Y_3MnCuS_7	*P*6_3	FM	$Y_2S_3 + Mn_2S_3 + CuS$	55.1221
Y_3FeTiS_7	*P*6_3	AFM1	$La_2S_3 + FeS_2 + FeS + TiS$	88.9613

Y_3FeVS_7	*P*6_3	AFM2	$La_2S_3 + FeS_2 + FeS + VS$	61.7225
Y_3FeCrS_7	*P*6_3	AFM2	$La_2S_3 + FeS_2 + FeS + CrS$	47.3885
Y_3FeMnS_7	*P*6_3	AFM2	$La_2S_3 + FeS_2 + FeS + MnS$	61.1164
Y_3FeFeS_7	*P*6_3	AFM2	$Y_2S_3 + FeS_2 + FeS$	128.1123
Y_3FeCoS_7	*P*6_3	AFM1	$La_2S_3 + FeS_2 + FeS + CoS$	123.6594
Y_3FeNiS_7	*P*6_3	AFM2	$La_2S_3 + FeS_2 + FeS + NiS$	126.2750
Y_3FeCuS_7	*P*6_3	FM	$La_2S_3 + FeS_2 + FeS + CuS$	99.7375
Y_3CoTiS_7	*P*6_3	AFM1	$La_2S_3 + Co_2S_3 + TiS$	35.9428
Y_3CoVS_7	*P*6_3	AFM1	$La_2S_3 + Co_2S_3 + VS$	68.3576
Y_3CoCrS_7	*P*6_3	AFM2	$La_2S_3 + Co_2S_3 + CrS$	30.7807
Y_3CoMnS_7	*P*6_3	AFM2	$La_2S_3 + Co_2S_3 + MnS$	80.7309
Y_3CoFeS_7	*P*6_3	FM	$La_2S_3 + Co_2S_3 + FeS$	136.7441
Y_3CoCoS_7	*P*6_3	AFM2	$Y_2S_3 + Co_2S_3 + CoS$	122.9027
Y_3CoNiS_7	*P*6_3	FM	$La_2S_3 + Co_2S_3 + NiS$	175.3139
Y_3CoCuS_7	*P*6_3	FM	$La_2S_3 + Co_2S_3 + CuS$	118.1625
Y_3NiTiS_7	*P*6_3	AFM1	$La_2S_3 + Ni_3S_4 + NiS_2 + TiS$	89.6707
Y_3NiVS_7	*P*6_3	AFM1	$La_2S_3 + Ni_3S_4 + NiS_2 + VS$	67.0390
Y_3NiCrS_7	*P*6_3	AFM2	$La_2S_3 + Ni_3S_4 + NiS_2 + CrS$	55.3778
Y_3NiMnS_7	*P*6_3	AFM2	$La_2S_3 + Ni_3S_4 + NiS_2 + MnS$	99.4790
Y_3NiFeS_7	*P*6_3	AFM1	$La_2S_3 + Ni_3S_4 + NiS_2 + FeS$	153.0025

Y_3NiCoS_7	*P*6_3	AFM1	$La_2S_3 + Ni_3S_4 + NiS_2 + CoS$	143.7661
Y_3NiNiS_7	*Pbam*	AFM1	$Y_2S_3 + Ni_3S_4 + NiS_2 + NiS$	108.6439
Y_3NiCuS_7	*P*6_3	AFM2	$Y_2S_3 + Ni_3S_4 + NiS_2 + CuS$	153.6791
Y_3CuTiS_7	*P*6_3	AFM1	Y_2S_3 + CuS_2(mp-849086) + CuS + TiS	-37.7696
Y_3CuVS_7	*P*6_3	FM	$Y_2S_3 + CuS_2 + CuS + VS$	36.2281
Y_3CuCrS_7	*P*6_3	AFM2	$Y_2S_3 + CuS_2 + CuS + CrS$	2.1575
Y_3CuMnS_7	*P*6_3	AFM2	$Y_2S_3 + CuS_2 + CuS + MnS$	46.5348
Y_3CuFeS_7	*P*6_3	AFM1	$Y_2S_3 + CuS_2 + CuS + FeS$	106.7750
Y_3CuCoS_7	*P*6_3	FM	$Y_2S_3 + CuS_2 + CuS + CoS$	92.8461
Y_3CuNiS_7	*P*6_3	FM	$Y_2S_3 + CuS_2 + CuS + NiS$	119.4819
Y_3CuCuS_7	*Pbam*	AFM1	$Y_2S_3 + CuS_2 + CuS$	120.5423

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