Supplementary Material

Unraveling conversion mechanism toward spinel sulfides as cathode materials for Mg-ion batteries

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Computational formula

The formation energies of magnesiated M_3S_4 at various Mg concentrations are expressed as equ (S1):

$$E_f = \frac{(E_{Mg_xM_3S_4} - E_{M_3S_4} - nE_{Mg})}{n}(M = Co / Ni) \quad \text{equ (S1)}$$

$E_{Mg_xM_3S_4}$, $E_{M_3S_4}$, E_{Mg} refer to the total energies of $Mg_xM_3S_4$, M_3S_4, and Mg, n represents the Mg ion concentration in the unit cell of M_3S_4 ($0 \le x \le 2$).

The voltage of the most stable $Mg_xM_3S_4$ configuration was calculated from first principles. The electrochemical reaction of battery discharge is shown in equ (S2):

$$M_3S_4 + xMg^{2+} + nxe^- \rightarrow Mg_xM_3S_4 \quad \text{equ (S2)}$$

The average voltage depends on the change of Gibbs free energy of the electrode. At the same time, because $p\Delta V$ and $T\Delta S$ are too small to be negligibled, the value of internal energy (ΔE) can represent the Gibbs free energy.

$$V = -[E_{Mg_{x_2}M_3S_4} - E_{Mg_{x_1}M_3S_4} - (x_2 - x_1)E_{Mg}] / (x_2 - x_1)z \quad \text{equ (S3)}$$

$E_{Mg_{x_2}M_3S_4}$, $E_{Mg_{x_1}M_3S_4}$, E_{Mg} represent the total energies of $Mg_{x_2}V_3S_4$, $Mg_{x_1}V_3S_4$, and each atom in metal Mg, x represents the number of metal ions Mg embedded in M_3S_4 ($0 \le x_1, 0 \le x_2 \le 2$), z is the charge transfer coefficient (z = 2 for Mg).

In order to expound the conversion mechanism, Ab initio molecular dynamics (AIMD) calculations were conducted in a

cubic 2× 2 × 2 supercell. The annealing process was performed at 300 K in a canonical ensemble for 2 ps with a time step of 1 fs. The local atomic arrangements in $Mg_xM_3S_4$ ($0 \leq x \leq 2$) can be characterized by the partial pair correlation function (PCF), in which $g_{AB}(r)$ represents the average number of B atoms for one species around A atoms for another species with the distance of r. Quantitatively, $g_{AB}(r)$ is calculated by equ (S4):

$$g_{AB}(r) = \frac{L^3}{N_A N_B} \frac{\sum_{A,B}^{N_A, N_B} n_{AB}(r)}{4\pi r^2 d_r} \qquad \text{equ (S4)}$$

where L is the length of the cubic unit cell, N_A and N_B are the numbers of A- and B-type atoms in the unit cell, respectively, and n_{AB} is the average number of B atoms around A atoms in the spherical shell of r - (r + dr).

Figure

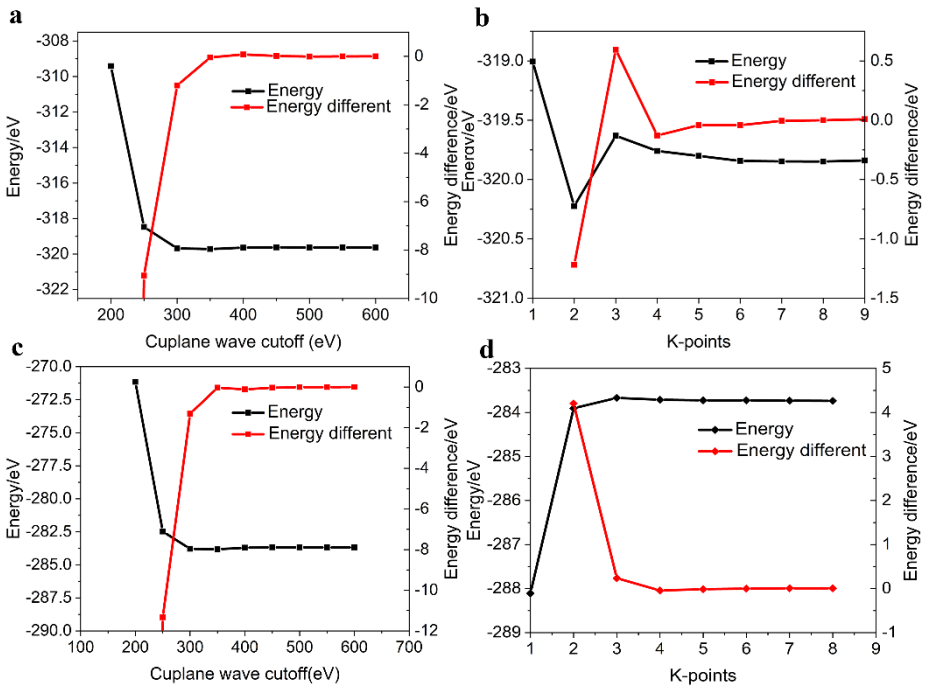

Fig. S1 (a) Relationship between different cutoff energies and energy of Co_3S_4, (b) Relationship between different K-points and energy of Co_3S_4 (c) Relationship between different cut-off energies and energy of Ni_3S_4, (d) Relationship between different K-points and energy of Ni_3S_4.

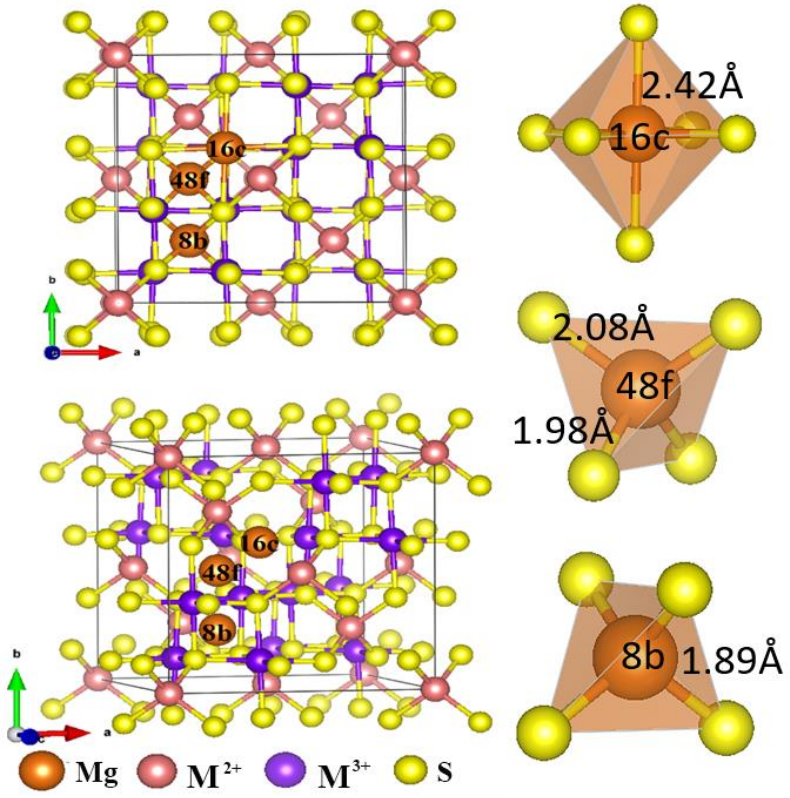

Fig. S2 Interstitial sites of M_3S_4 crystal.

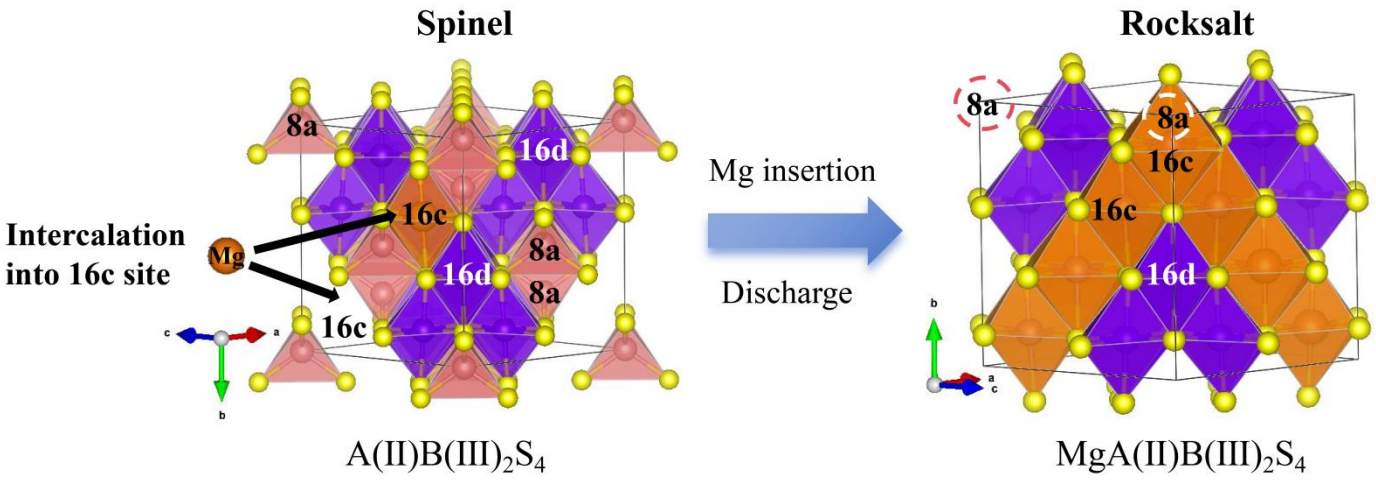

Fig. S3 Transformation of spinel phase to rock salt phase during the magnesiation.

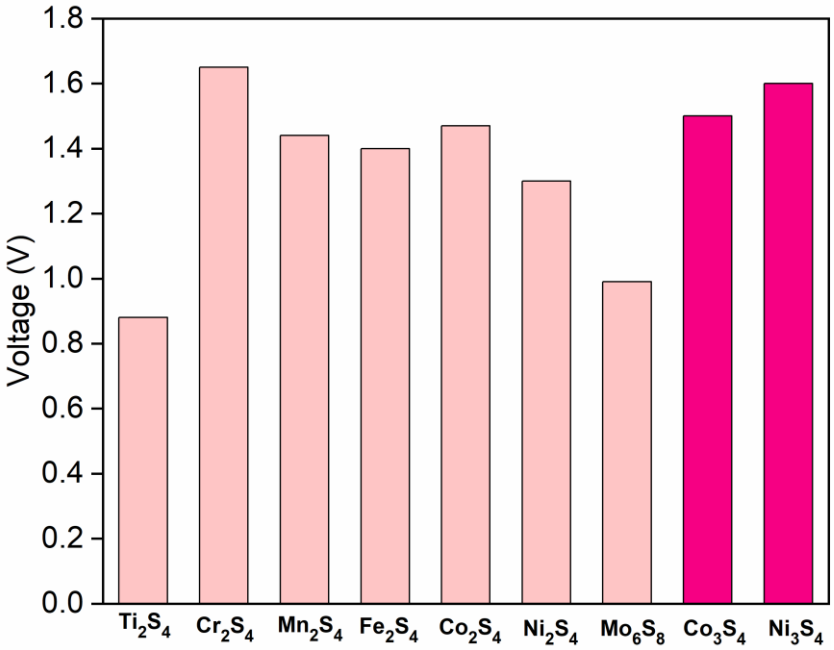

Fig. S4 Comparison between the discharge voltages of the spinel sulfides and other transition metal sulfides as cathode materials for Mg batteries.

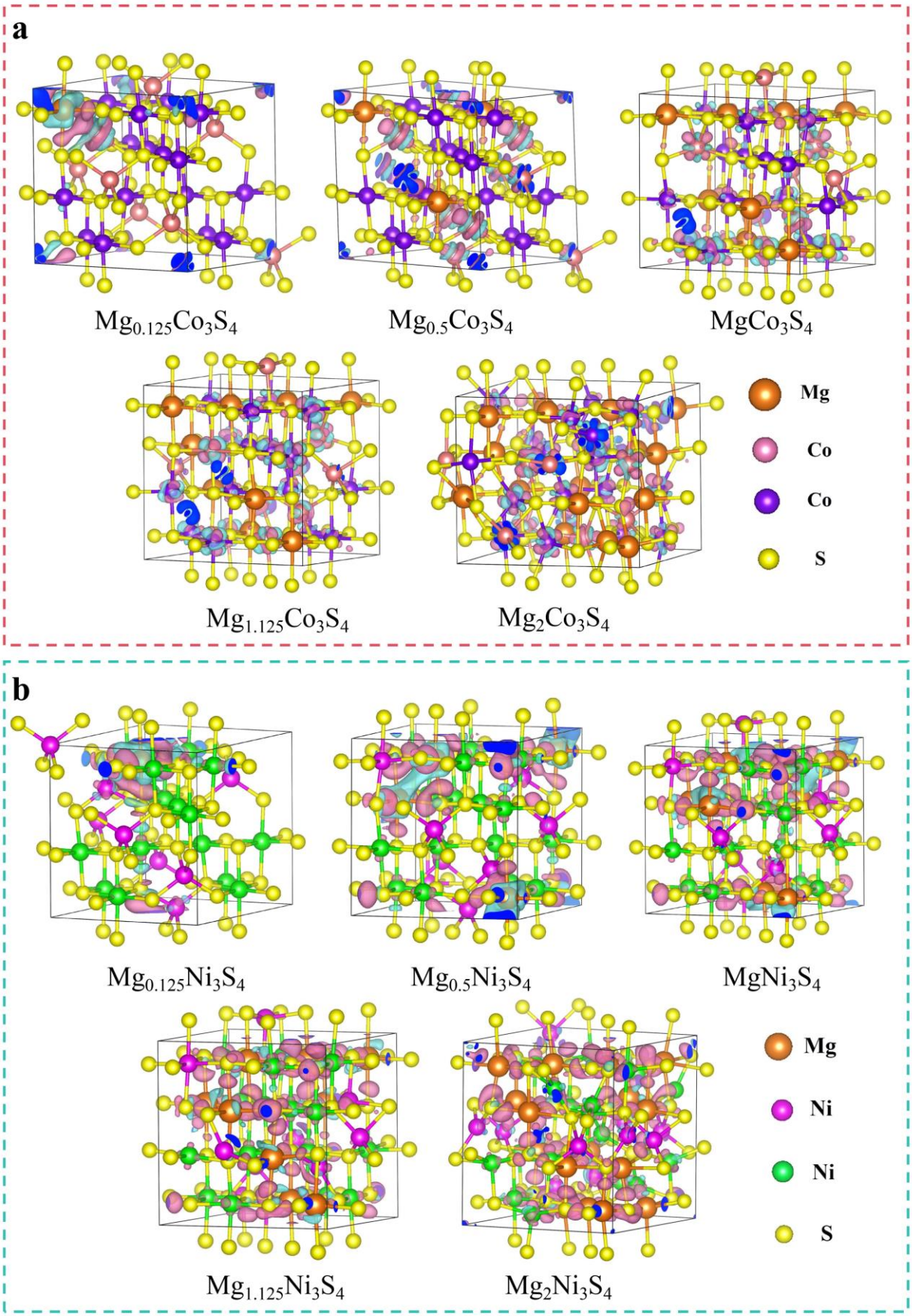

Fig. S5 Differential charge densities of (a) $Mg_xCo_3S_4$ and (b) $Mg_xNi_3S_4$ at. Pink (blue) is the spatial regions gain (loss) in charge.

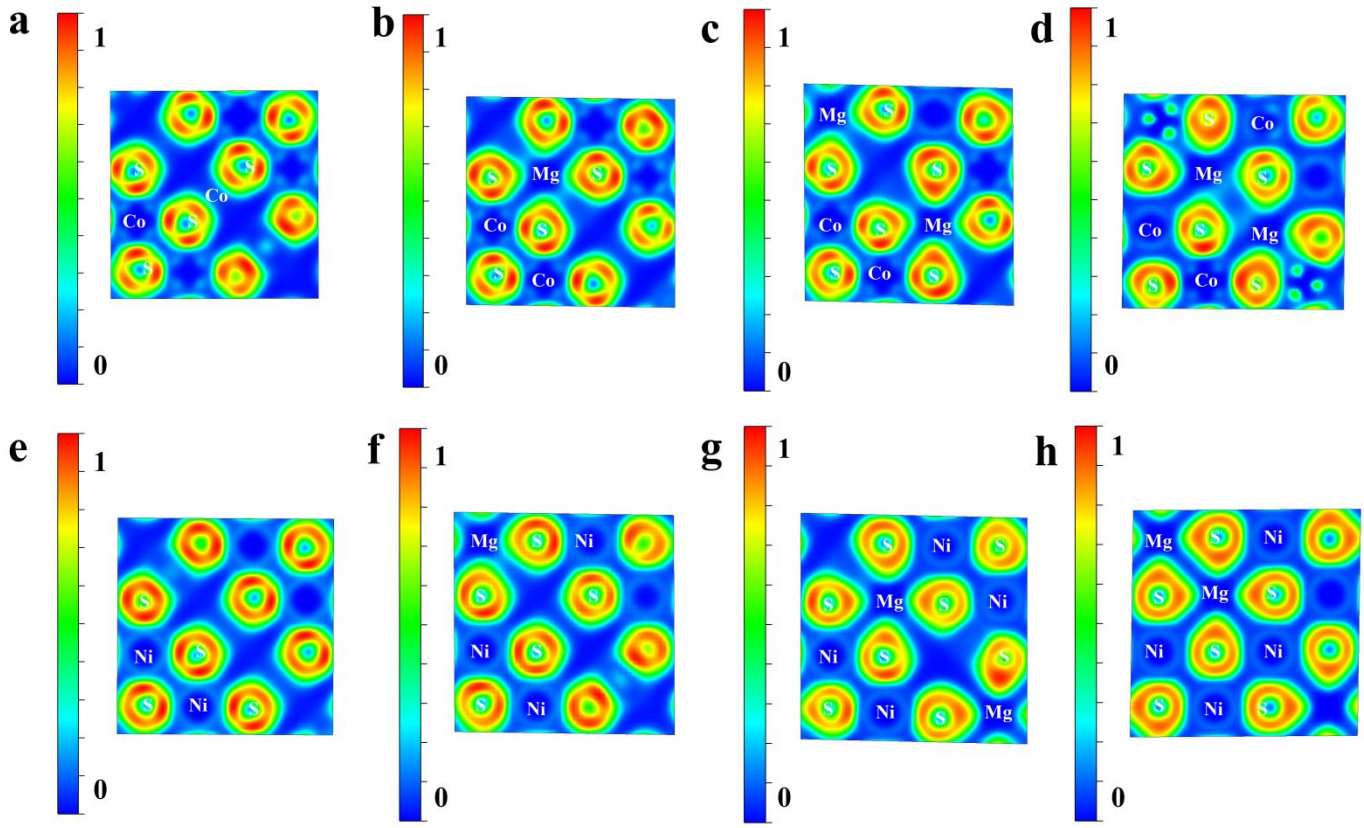

Fig. S6 Electronic localization function (ELF) diagrams of (a) Co_3S_4, (b) $Mg_{0.125}Co_3S_4$, (c) $Mg_{0.625}Co_3S_4$, (d) $MgCo_3S_4$ and (e) Ni_3S_4, (f) $Mg_{0.125}Ni_3S_4$, (g) $Mg_{0.625}Ni_3S_4$, (h) $MgNi_3S_4$.

Tables

Table S1 Lattice parameters of Ni_3S_4 before and after structural optimization.

Ni_3S_4	a(Å)	b(Å)	c(Å)	α	β	γ	V(Å^3)
Experiment values	9.457	9.457	9.457	90°	90°	90°	845.78
Optimized values	9.330	9.330	9.330	90°	90°	90°	812.29
E_r	-1.34%	-1.34%	-1.34%	0%	0%	0%	-3.96%

Table S2 Lattice parameters of Co_3S_4 before and after structural optimization.

Co_3S_4	a(Å)	b(Å)	c(Å)	α	β	γ	V(Å^3)
Experiment values	9.401	9.401	9.401	90°	90°	90°	830.85
Optimized values	9.501	9.501	9.501	90°	90°	90°	857.844
Er	1.06%	1.06%	1.06%	0.00%	0.00%	0.00%	3.2%

Table S3 Wyckoff sites of M_3S_4

Elements	Wyckoff sites	Fractional coordinates (x, y, z)
M1	*8a*	(0, 0, 0)
M2	*16d*	(0.625, 0.625, 0.625)
S	*32e*	(-0.135, -0.135, -0.135)

Table S4 Energies and volumetric expansion ratio of $Mg_{0.125}Co_3S_4$ at different interstitials sites

Interstitials sites	Energies/eV	Volumetric expansion ratio/%
16c	-272.99178	0.76%
48f	-271.53713	2.16%
8b	-268.06943	4.11%

Table S5 Energies and volumetric expansion ratio of $Mg_{0.125}Ni_3S_4$ at different interstitials sites.

Interstitials sites	Energies/eV	Volumetric expansion ratio/%
16c	-239.56708 eV	6.82%
48f	-238.68149 eV	7.20%
8b	-235.34990 eV	7.93%

It can be calculated from Table S3 that the formation energies of 16c, 48f, and 8b vacancies are -1.08 eV, -0.38 eV, and 3.85 eV, respectively. From Table S4, the formation energies of 16c, 48f, and 8b vacancies are calculated to be -2.06 eV，-1.17 eV，2.16 eV, respectively. The three configurations are stable after structural relaxation, but they all have the lowest formation energy at the 16c site and have the most stable structure, so Mg^{2+} is preferentially embedded in the octahedral 16c site.

Table S6 Energies, Formation energy and Volumetric expansion ratios of $Mg_xCo_3S_4$ at different Mg concentrations.

Molecular formula	Energies (eV)	Formation energies (eV)	Volumetric expansion ratios
Co_3S_4	-270.41250	-	0%
$Mg_{0.125}Co_3S_4$	-275.71632	-1.08	0.76%
$Mg_{0.625}Co_3S_4$	-284.41889	-1.29	5.52%
$MgCo_3S_4$	-303.43320	-2.62	18.98%
$Mg_{1.25}Co_3S_4$	-315.52613	-3.01	23.19%
$Mg_2Co_3S_4$	-332.09019	-2.23	36.95%

Table S7 Energies, Formation energy and Volumetric expansion ratios of $Mg_xNi_3S_4$ at different Mg concentrations.

Molecular formula	Energies (eV)	Formation energy (eV)	Volumetric expansion ratios
Ni_3S_4	-236.00625	-	0%
$Mg_{0.125}Ni_3S_4$	-239.56708	-2.06	6.82%
$Mg_{0.625}Ni_3S_4$	-257.06390	-2.71	15.58%
$MgNi_3S_4$	-271.56967	-2.94	20.72%
$Mg_{1.25}Ni_3S_4$	-280.75009	-2.97	23.6%
$Mg_2Ni_3S_4$	-293.666378	-2.10	35.02%

Table S8 Lattice parameters of $Mg_xCo_3S_4$ at different Mg concentrations.

Molecular formula	a(Å)	b(Å)	c(Å)	α	β	γ	V(Å^3)
Co_3S_4	9.501	9.501	9.501	90.0°	90.0°	90.0°	857.844
$Mg_{0.125}Co_3S_4$	9.526	9.526	9.526	90.0°	90.0°	90.0°	864.354
$Mg_{0.625}Co_3S_4$	9.500	9.858	9.692	86.6°	91.2°	81.7°	905.195
$MgCo_3S_4$	10.036	10.106	10.067	89.3°	90.5°	91.6°	1020.723
$Mg_{1.25}Co_3S_4$	10.081	10.229	10.247	89.5	90.2	90.1	1056.731
$Mg_2Co_3S_4$	11.191	11.229	9.356	89.7°	88.7°	88.0°	1174.798
$Mg_3Co_3S_4$	10.877	10.877	10.877	90	90	90	1287.043

Table S9 Lattice parameters of $Mg_xNi_3S_4$ at different Mg concentrations.

Molecular formula	a(Å)	b(Å)	c(Å)	α	β	γ	V(Å^3)
Ni_3S_4	9.330	9.330	9.330	90°	90°	90°	812.292
$Mg_{0.125}Ni_3S_4$	9.539	9.539	9.539	90°	90°	90°	867.719
$Mg_{0.625}Ni_3S_4$	9.777	9.806	9.800	88.9°	91.4°	91.3°	905.195
$MgNi_3S_4$	9.952	9.948	0.906	88.7°	90°	90.3°	980.562
$Mg_{1.25}Ni_3S_4$	9.970	10.038	10.033	89.9	90	89.9	1004.229
$Mg_2Ni_3S_4$	11.083	10.256	9.376	89.3°	88.9°	88.2°	1096.757
$Mg_3Ni_3S_4$	10.835	10.835	10.835	90	90	90	1272.221

Table S10 Specific capacities and Energy densities of $Mg_xM_3S_4$ at different Mg concentrations.

Systems	Co_3S_4	$Mg_{0.125}Co_3S_4$	$Mg_{0.625}Co_3S_4$	$MgCo_3S_4$	$Mg_{1.25}Co_3S_4$	$Mg_2Co_3S_4$	$Mg_3Co_3S_4$
Specific capacity/mAh • g^{-1}	702.80	21.96	109.83	175.72	219.66	351.45	527.18
Energy density/Wh • kg^{-1}	-	32.94	164.74	263.59	329.49	221.41	332.12

Table S11 Specific capacities and Energy densities of $Mg_xM_3S_4$ at different Mg concentrations.

Systems	Ni_3S_4	$Mg_{0.125}Ni_3S_4$	$Mg_{0.625}Ni_3S_4$	$MgNi_3S_4$	$Mg_{1.25}Ni_3S_4$	$Mg_2Ni_3S_4$	$Mg_3Ni_3S_4$
Specific capacity/mAh • g^{-1}	704.50	22.01	110.41	176.66	220.83	353.33	538.43
Energy density/Wh • kg^{-1}	-	35.23	176.66	282.66	353.33	247.33	369.90

Table S12 Comparison of Mg diffusion barriers in spinel sulfides.

Molecular formula	Migration paths	Diffusion Barrier (eV)
Cr_2S_4[1]	8a-16c-8a	0.542
$MgSn_2S_4$[2]	8a-16c-8a	0.590
Ti_2S_4[1]	16c-8a-16c	0.615
Mn_2S_4[1]	16c-8a-16c	0.515
TiS_2[3]	16c-8a-16c	0.700
NiS_2[3]	16c-8a-16c	0.460
Co_3S_4[This work]	**16c-48f-16c**	**1.100**
Ni_3S_4[This work]	**16c-48f-16c-48f-16c**	**0.670**

Table S13 Average Bader charge values of Mg, Co and S for $Mg_xCo_3S_4$ ($0 \le x \le 2$).

Molecular formula	Mg (e^-)	Co (e^-)	S (e^-)
Co_3S_4	-	0.70	-0.52
$Mg_{0.125}Co_3S_4$	1.57	0.64	-0.53
$Mg_{0.625}Co_3S_4$	1.57	0.59	-0.69
$MgCo_3S_4$	1.60	0.81	-1.01
$Mg_{1.25}Co_3S_4$	1.60	0.84	-1.13
$Mg_2Co_3S_4$	1.60	0.56	-1.22
$Mg_3Co_3S_4$	1.54	-0.04	-1.12

Table S14 Average Bader charge values of Mg, Ni and S for $Mg_xNi_3S_4$ ($0 \le x \le 2$).

Molecular formula	Mg (e^-)	Ni (e^-)	S (e^-)
Ni_3S_4	-	0.50	-0.38
$Mg_{0.125}Ni_3S_4$	1.56	0.53	-0.44
$Mg_{0.625}Ni_3S_4$	1.58	0.64	-0.73
$MgNi_3S_4$	1.58	0.51	-0.78
$Mg_{1.25}Ni_3S_4$	1.59	0.71	-1.03
$Mg_2Ni_3S_4$	1.58	0.30	-1.02
$Mg_3Ni_3S_4$	1.58	0.04	-1.22

Table S15 Bader charge values of $Mg_xCo_3S_4$ per atom.

Atoms	Co_3S_4 (e^-)	$Mg_{0.125}Co_3S_4$ (e^-)	$Mg_{0.625}Co_3S_4$ (e^-)	$MgCo_3S_4$ (e^-)	$Mg_{1.25}Co_3S_4$ (e^-)	$Mg_2Co_3S_4$ (e^-)	$Mg_3Co_3S_4$ (e^-)
Co1	0.83084	0.84267	0.50767	0.90663	0.88375	0.44776	-0.08895
Co2	0.83084	0.84267	0.50786	0.84524	0.37558	0.54915	0.11218
Co3	0.83084	0.47256	0.41844	0.89367	0.88328	0.38038	0.12158
Co4	0.83084	0.84267	0.57046	0.85173	0.56583	0.43132	-0.04071
Co5	0.83084	0.84267	0.53174	0.46712	0.89554	0.49758	-0.05500
Co6	0.83084	0.84267	0.50983	0.51189	0.37977	0.39238	-0.39005
Co7	0.83084	0.47256	0.5041	0.46903	0.93093	0.07766	-0.13993
Co8	0.83084	0.84267	0.41928	0.50607	0.48038	0.21751	0.03679
Co9	0.63603	0.53437	0.612	0.76958	0.94548	0.51624	-0.32063

Co10	0.63288	0.53437	0.66386	0.93145	0.85707	0.82392	-0.00845
Co11	0.63288	0.47622	0.64125	0.91487	0.92533	0.72696	0.02616
Co12	0.63288	0.53437	0.67752	0.94061	0.94339	0.95181	-0.29967
Co13	0.63288	0.67871	0.6663	0.93678	0.89154	0.27845	0.37344
Co14	0.63288	0.53617	0.62	0.93867	0.93184	0.48066	0.14327
Co15	0.63288	0.67871	0.66712	0.93000	0.91474	0.31761	-0.01577
Co16	0.63128	0.67871	0.62053	0.93142	0.86496	0.25668	0.13480
Co17	0.63131	0.53437	0.69066	0.72760	0.92877	0.38019	-0.26994
Co18	0.63603	0.53617	0.65345	0.93489	0.93076	0.93997	0.15977
Co19	0.63603	0.67871	0.68764	0.73673	0.97287	0.77422	-0.24945
Co20	0.63131	0.53617	0.65944	0.73926	0.93752	0.94590	-0.05538
Co21	0.63128	0.53437	0.61205	0.89493	0.91912	0.48093	-0.19402
Co22	0.63131	0.67871	0.66089	0.94311	0.94622	0.80865	-0.13668
Co23	0.63603	0.53437	0.66147	0.94587	0.91757	0.82747	-0.02613
Co24	0.63131	0.67871	0.58606	0.77153	0.93545	0.93464	0.17802
S1	-0.52336	-0.50737	-0.71661	-1.14164	-1.15605	-1.13096	-1.3803
S2	-0.52336	-0.50737	-0.73981	-0.97736	-1.04491	-1.2529	-1.0906
S3	-0.52336	-0.50798	-0.89589	-1.19313	-1.13677	-1.40938	-0.97482
S4	-0.52336	-0.50737	-0.49762	-0.70108	-1.16117	-1.12356	-1.24622
S5	-0.52336	-0.50737	-0.7327	-1.14506	-1.27191	-1.20055	-1.19373
S6	-0.52808	-0.50737	-0.7041	-0.83564	-1.02715	-1.16900	-0.95423
S7	-0.52336	-0.50798	-0.74072	-0.75811	-1.17894	-1.31961	-1.10889
S8	-0.52336	-0.50737	-0.71223	-1.02553	-0.97078	-1.02678	-0.93060
S9	-0.52336	-0.6444	-0.71277	-1.08703	-1.15773	-1.11734	-1.29210
S10	-0.52336	-0.5096	-0.89914	-1.17274	-1.14708	-1.04652	-1.27207
S11	-0.52336	-0.48424	-0.50251	-0.7733	-1.17892	-1.31428	-0.82405
S12	-0.52336	-0.48424	-0.74425	-1.02678	-1.15024	-1.31420	-1.10755
S13	-0.52336	-0.5096	-0.69088	-0.83106	-1.0173	-1.32468	-1.20798
S14	-0.52336	-0.6444	-0.71542	-1.18732	-1.1518	-1.29074	-1.56905
S15	-0.52339	-0.48424	-0.68946	-1.00134	-0.97152	-1.35032	-0.77179
S16	-0.52493	-0.50737	-0.67818	-1.18537	-1.27038	-1.27209	-1.25655
S17	-0.52651	-0.5096	-0.69634	-0.83556	-1.25045	-1.32728	-0.82430

S18	-0.52336	-0.50737	-0.92996	-0.99830	-1.14325	-1.29276	-1.28352
S19	-0.52493	-0.6444	-0.68572	-1.12306	-1.25445	-1.14909	-0.75332
S20	-0.52336	-0.5096	-0.71416	-1.17180	-1.17251	-1.27258	-1.26114
S21	-0.52339	-0.48424	-0.7351	-1.08620	-1.17999	-1.24507	-1.31511
S22	-0.52493	-0.5096	-0.68746	-0.76357	-1.16732	-1.09005	-0.92875
S23	-0.52811	-0.6444	-0.92073	-1.18635	-1.27445	-1.16539	-1.02342
S24	-0.52493	-0.5096	-0.75258	-1.18762	-1.14999	-1.16755	-0.94584
S25	-0.52339	-0.50737	-0.67096	-0.96819	-1.1106	-1.27999	-1.16761
S26	-0.52493	-0.48424	-0.55999	-1.18551	-1.1291	-1.39369	-1.37835
S27	-0.52493	-0.50737	-0.64973	-1.14740	-1.12518	-1.26923	-1.01538
S28	-0.52654	-0.6444	-0.48317	-0.76736	-1.18277	-0.95479	-1.01567
S29	-0.52336	-0.50737	-0.55748	-1.03683	-0.95776	-1.13216	-1.08631
S30	-0.52493	-0.50737	-0.48178	-0.69876	-0.87673	-1.32272	-1.46589
S31	-0.52339	-0.6444	-0.65593	-1.12819	-1.15111	-1.08695	-1.19612
S32	-0.52493	-0.48424	-0.67951	-0.88062	-1.01288	-1.20027	-1.07342
Mg1	-	1.5695	1.57295	1.59948	1.59703	1.61367	1.53448
Mg2	-	-	1.57343	1.59015	1.59505	1.57540	1.53652
Mg3	-	-	1.56973	1.59974	1.59742	1.59959	1.55058
Mg4	-	-	1.57126	1.58947	1.60148	1.60755	1.54424
Mg5	-	-	1.59588	1.59966	1.596	1.60481	1.53692
Mg6	-	-	-	1.60259	1.59569	1.60655	1.53971
Mg7	-	-	-	1.59261	1.59917	1.59962	1.54348
Mg8	-	-	-	1.59541	1.59626	1.60288	1.54468
Mg9	-	-	-	-	1.59425	1.59292	1.55027
Mg10	-	-	-	-	1.60112	1.58343	1.52205
Mg11	-	-	-	-	-	1.60310	1.53788
Mg12	-	-	-	-	-	1.58872	1.56024
Mg13	-	-	-	-	-	1.59849	1.48460
Mg14	-	-	-	-	-	1.60506	1.57811
Mg15	-	-	-	-	-	1.59285	1.52154
Mg16	-	-	-	-	-	1.59982	1.51191
Mg17	-	-	-	-	-	-	1.54251

Mg18	-	-	-	-	-	-	1.53839
Mg19	-	-	-	-	-	-	1.56600
Mg20	-	-	-	-	-	-	1.55701
Mg21	-	-	-	-	-	-	1.53693
Mg22	-	-	-	-	-	-	1.52339
Mg23	-	-	-	-	-	-	1.53022
Mg24	-	-	-	-	-	-	1.52779

Table S16 Bader charge values of $Mg_xNi_3S_4$ per atom.

Atoms	**Ni_3S_4 (e^-)**	**$Mg_{0.125}Ni_3S_4$ (e^-)**	**$Mg_{0.625}Ni_3S_4$ (e^-)**	**$MgNi_3S_4$ (e^-)**	**$Mg_{1.25}Ni_3S_4$ (e^-)**	**$Mg_2Ni_3S_4$ (e^-)**	**$Mg_3Ni_3S_4$ (e^-)**
Ni1	0.45654	0.39292	0.62747	0.50068	0.82897	0.18820	-0.13914
Ni2	0.45654	0.64179	0.57945	0.21657	0.76935	0.09938	-0.02969
Ni3	0.45654	0.64179	0.63681	0.48724	0.22926	0.04022	0.07450
Ni4	0.45654	0.6354	0.44397	0.33240	0.26967	0.01402	-0.05994
Ni5	0.45654	0.39292	0.50111	0.46886	0.38399	0.21543	-0.02948
Ni6	0.45654	0.5548	0.47867	0.20902	0.78001	-0.02011	-0.12823
Ni7	0.45654	0.33984	0.46896	0.50652	0.27882	0.46094	0.02650
Ni8	0.45654	0.64179	0.41702	0.44179	0.75	0.36238	-0.15108
Ni9	0.53066	0.5548	0.76848	0.51865	0.75359	0.60937	0.08506
Ni10	0.52778	0.6354	0.61514	0.56499	0.81897	0.01371	0.11889
Ni11	0.52778	0.33984	0.72846	0.61079	0.76289	0.39451	0.11303
Ni12	0.52778	0.64179	0.71728	0.50510	0.73147	0.54179	0.08481
Ni13	0.52778	0.39292	0.66064	0.57773	0.82449	0.13614	0.02311
Ni14	0.52778	0.5548	0.5965	0.62424	0.75115	0.40701	0.14300
Ni15	0.52778	0.64179	0.78428	0.56068	0.86127	0.47218	0.0706
Ni16	0.52632	0.6354	0.58837	0.52824	0.80884	0.04571	0.05273
Ni17	0.52635	0.39292	0.70227	0.60776	0.75881	0.51849	0.19893
Ni18	0.53066	0.64179	0.68335	0.59473	0.76429	0.42383	-0.0037
Ni19	0.53066	0.39292	0.7361	0.61269	0.81391	0.44167	-0.41092
Ni20	0.52632	0.5548	0.69618	0.60088	0.86952	0.41886	0.29024
Ni21	0.52632	0.5548	0.7177	0.57397	0.83291	0.19900	0.26303

Ni22	0.52635	0.53904	0.75151	0.59730	0.886	0.50269	0.06088
Ni23	0.53066	0.39292	0.71904	0.55330	0.76338	0.49431	0.37346
Ni24	0.52635	0.5548	0.77838	0.56537	0.7831	0.17010	-0.01808
S1	-0.38164	-0.36044	-0.80954	-0.70541	-1.20881	-0.71980	-0.92496
S2	-0.37730	-0.37269	-1.03364	-0.60749	-1.10744	-0.89407	-0.92359
S3	-0.37730	-0.36044	-0.43924	-0.94019	-0.83599	-1.22852	-1.50537
S4	-0.37730	-0.37269	-0.4528	-0.67246	-0.80612	-1.16925	-1.41662
S5	-0.37730	-0.46161	-0.43918	-0.91482	-1.02248	-1.01551	-1.34148
S6	-0.37730	-0.46161	-0.76337	-0.58867	-1.10945	-0.94723	-0.94476
S7	-0.37730	-0.37269	-0.98838	-0.96102	-1.06866	-1.35753	-1.08782
S8	-0.37730	-0.36044	-0.53899	-0.45594	-0.99659	-1.15009	-1.32869
S9	-0.37730	-0.70347	-0.96715	-0.92759	-1.15694	-0.90256	-1.44547
S10	-0.37730	-0.70347	-0.67654	-0.48193	-1.07375	-1.39486	-1.17213
S11	-0.37730	-0.70347	-0.72647	-0.93420	-1.17717	-0.64739	-1.42738
S12	-0.37730	-0.70347	-0.70429	-0.43849	-1.06827	-0.86283	-1.20050
S13	-0.37730	-0.33768	-1.17922	-0.80821	-1.16946	-1.05232	-1.35871
S14	-0.37730	-0.46161	-0.53773	-0.93455	-1.08408	-1.12188	-0.94946
S15	-0.37733	-0.36044	-0.9847	-0.58346	-1.04987	-1.30275	-1.31989
S16	-0.37874	-0.70347	-0.70568	-0.97569	-1.06972	-0.75252	-0.87330
S17	-0.37874	-0.36044	-0.87386	-0.69086	-0.97429	-0.79471	-1.20697
S18	-0.38018	-0.36044	-0.85434	-0.47441	-0.96123	-0.90267	-1.25683
S19	-0.37874	-0.36044	-0.66877	-0.94151	-0.98114	-0.93977	-0.77126
S20	-0.37730	-0.36044	-0.6735	-0.79273	-1.07066	-1.30661	-0.81701
S21	-0.37733	-0.46161	-0.76436	-0.60728	-0.99321	-1.24641	-1.47820
S22	-0.38018	-0.46161	-0.75074	-0.96942	-1.02388	-1.16271	-1.34247
S23	-0.38018	-0.36044	-0.62407	-0.90692	-0.79892	-0.71580	-1.01957
S24	-0.37874	-0.37269	-0.72761	-0.72309	-1.03869	-0.91872	-1.58500
S25	-0.37730	-0.37269	-0.71842	-0.57707	-0.83969	-0.95947	-1.50884
S26	-0.37874	-0.36044	-0.56183	-0.90692	-1.05898	-1.35809	-1.1327
S27	-0.37874	-0.37269	-0.73402	-1.10686	-1.01952	-1.08714	-1.26206
S28	-0.3802	-0.36044	-0.74529	-1.14612	-1.01813	-0.79343	-0.95413
S29	-0.37730	-0.46161	-0.43823	-0.79783	-1.00556	-1.05689	-1.2014

S30	-0.37730	-0.33768	-0.97867	-0.79667	-1.08953	-1.13268	-1.43673
S31	-0.37733	-0.70347	-0.49359	-1.12212	-0.99396	-0.57906	-1.39001
S32	-0.37874	-0.36044	-0.76417	-0.49487	-1.1433	-1.00974	-1.45622
Mg1	-	1.56525	1.58324	1.57332	1.59395	1.55444	1.55402
Mg2	-	-	1.58723	1.57479	1.5944	1.59732	1.58452
Mg3	-	-	1.58075	1.58109	1.58861	1.56400	1.59001
Mg4	-	-	1.58812	1.58337	1.59496	1.59357	1.57041
Mg5	-	-	1.58189	1.58034	1.59223	1.59851	1.57875
Mg6	-	-	-	1.57354	1.59669	1.57761	1.59737
Mg7	-	-	-	1.57643	1.59883	1.58803	1.58184
Mg8	-	-	-	1.58243	1.59477	1.56552	1.59123
Mg9	-	-	-	-	1.59326	1.58393	1.54358
Mg10	-	-	-	-	1.59307	1.58632	1.59753
Mg11	-	-	-	-	-	1.59351	1.57922
Mg12	-	-	-	-	-	1.59646	1.58671
Mg13	-	-	-	-	-	1.57750	1.60306
Mg14	-	-	-	-	-	1.57209	1.58762
Mg15	-	-	-	-	-	1.59188	1.58573
Mg16	-	-	-	-	-	1.59249	1.59383
Mg17	-	-	-	-	-	-	1.56631
Mg18	-	-	-	-	-	-	1.58955
Mg19	-	-	-	-	-	-	1.60306
Mg20	-	-	-	-	-	-	1.58548
Mg21	-	-	-	-	-	-	1.58318
Mg22	-	-	-	-	-	-	1.60369
Mg23	-	-	-	-	-	-	1.56614
Mg24	-	-	-	-	-	-	1.60816

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