Supporting Information

First principles investigation of anionic redox in bisulfate lithium battery cathodes

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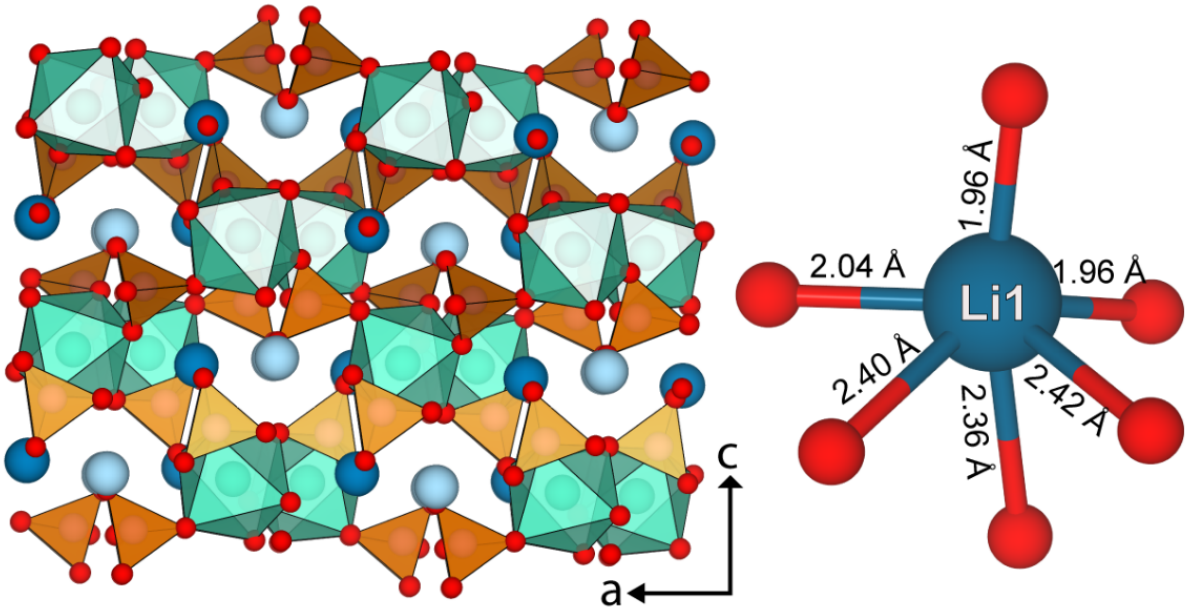

Figure S1. Crystal framework of orthorhombic (o)-$Li_2M(SO_4)_2$ along *b* direction. Dark and light blue spheres represent Li1 and Li2 sites. Orange and cyan polyhedra indicate the SO_4 tetrahedra and MO_6 octahedra. Right panel represents the distorton in LiO_6 octahedra of Li1 sites.

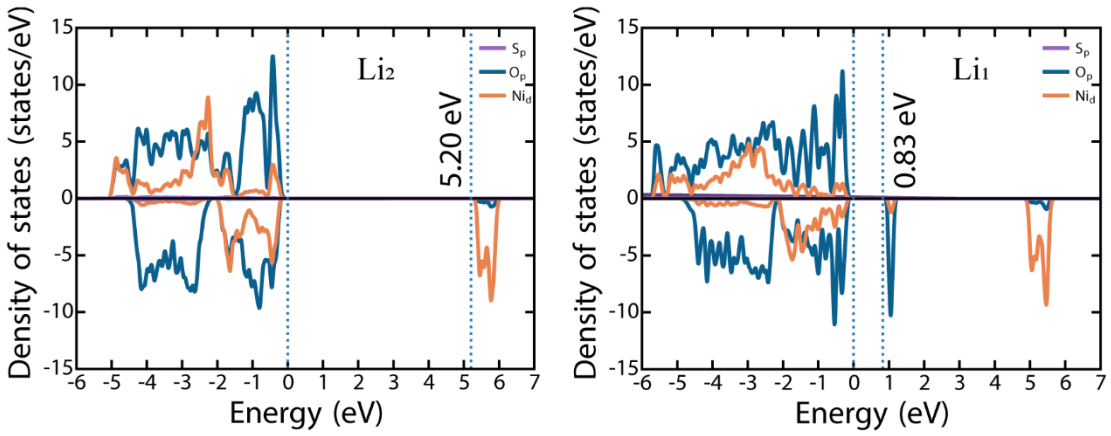

Figure S2. Hybrid functional calculated projected density of states (pDOS) for monoclinic (m)-$Li_2Ni(SO_4)_2$ and $LiNi(SO4)_2$ in left and right panel respectively. Purple, blue, and orange curves represent S *p*, O *p*, and Ni *d* states respectively. Dotted blue lines indicate the valence and conduction band edges, with the numbers indicating band gap values.

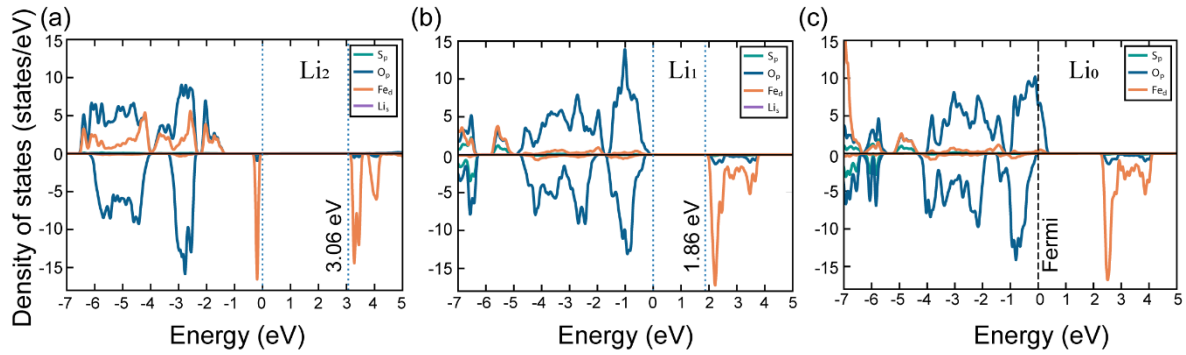

Figure S3. Projected density of state (pDOS) for monoclinic m-$Li_xFe(SO_4)_2$ at different states of (de)lithiation, namely x = 2, 1, and 0, as calculated by the Hubbard *U* corrected strongly constrained and appropriately normed (SCAN+*U*) functional. Cyan, blue, orange, and purple curves correspond to S *p*, O *p*, Fe *d*, and Li *s* states respectively. Dotted blue lines represent the valence and conduction band edges, while dashed black line indicates the Fermi level. Band gaps are indicated by the text notations at the corresponding conduction band minima.

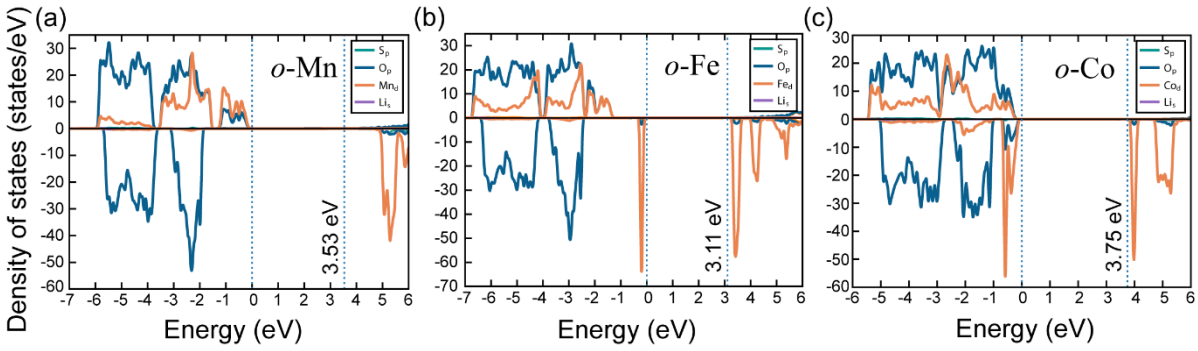

Figure S4. SCAN+*U*-calculated pDOS for o-$Li_2M(SO_4)_2$, where M = Mn, Fe and Co in panels a, b, and c, respectively. Notations on each panel are identical to **Figure S3**.

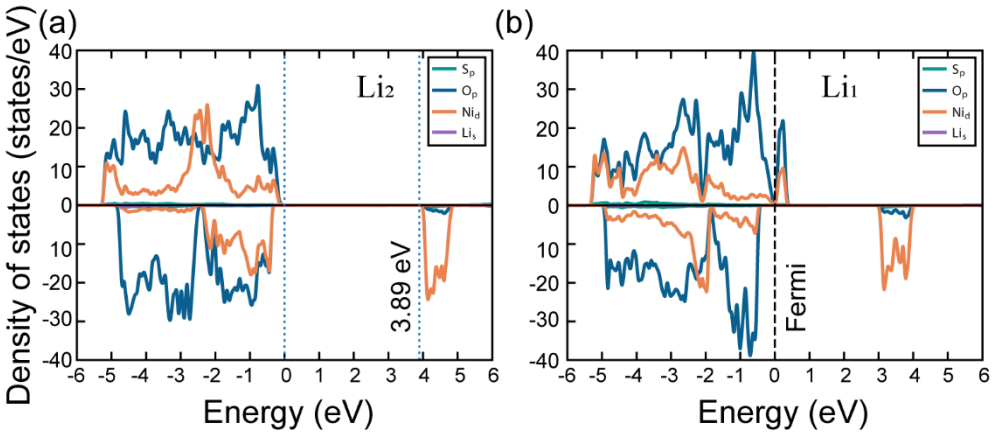

Figure S5. SCAN+*U*-calculated pDOS of o-$Li_xNi(SO_4)_2$ for x = 2 (panel a) and 1 (panel b). Notations on each panel are identical **Figure S3**.

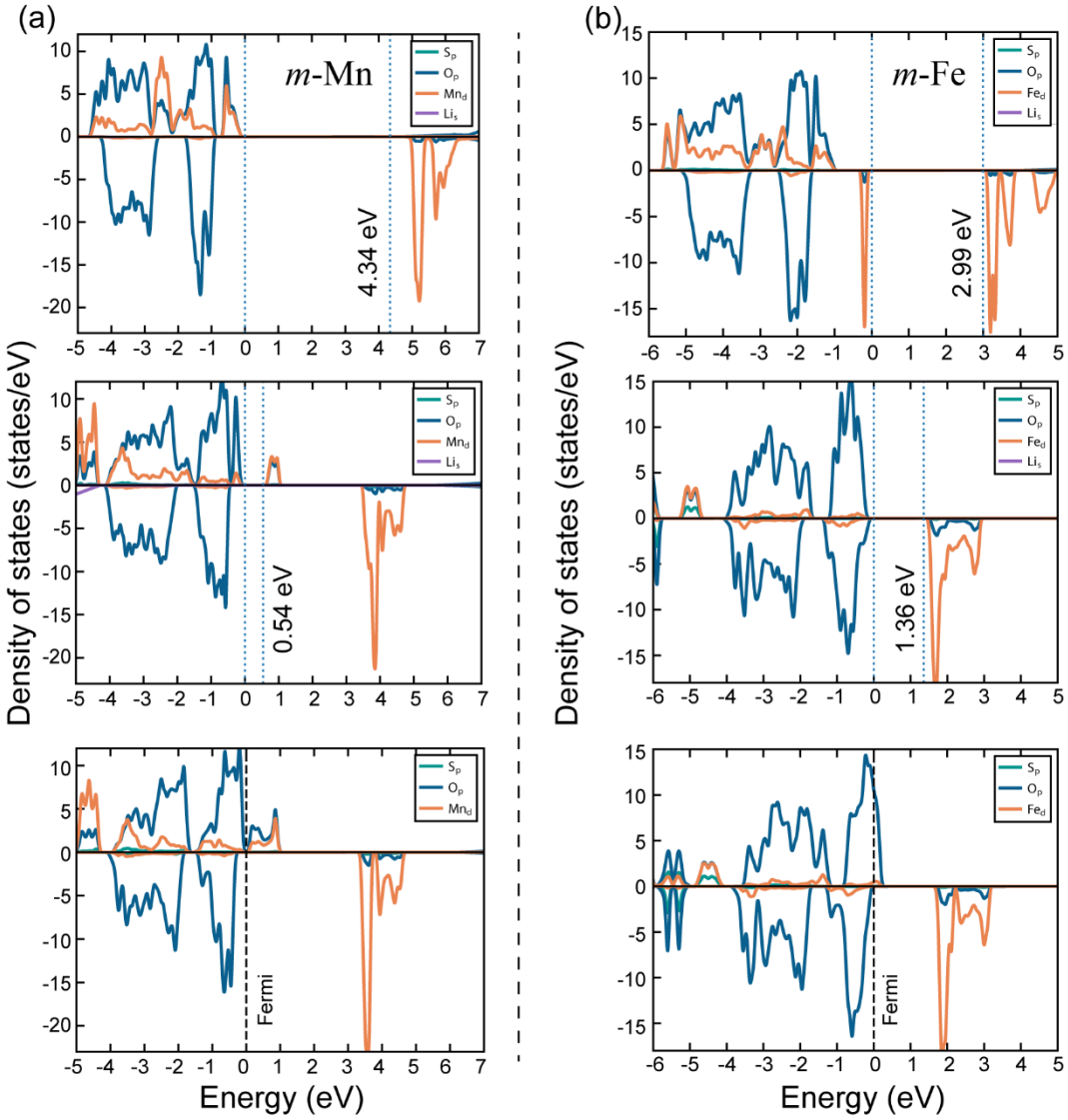

Figure S6. Hubbard *U* corrected generalized gradient approximation (GGA+*U*)-calculated pDOS of (a) m-$Li_xMn(SO_4)_2$ and (b) m-$Li_xFe(SO_4)_2$. Top, middle, and bottom panels represent different levels of (de)lithiation, namely, x = 2, 1, and 0, respectively. Notations on each panel are identical to **Figure S3.**

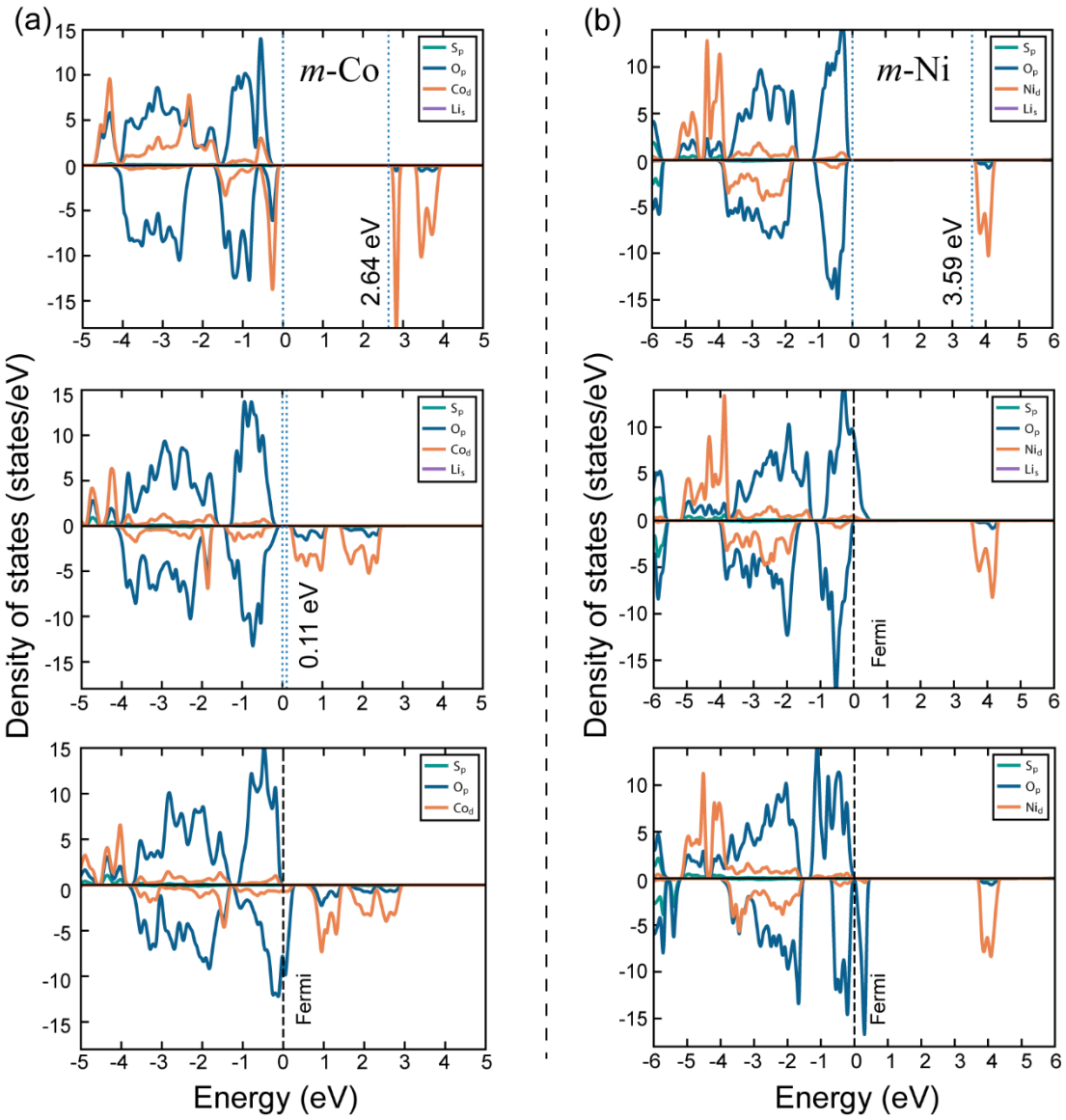

Figure S7. GGA+*U*-calculated pDOS of (a) m-$Li_xCo(SO_4)_2$ and (b) m-$Li_xNi(SO_4)_2$. Top, middle, and bottom panels represent different levels of (de)lithiation, namely, x = 2, 1, and 0, respectively. Notations on each panel are identical to **Figure S3.**

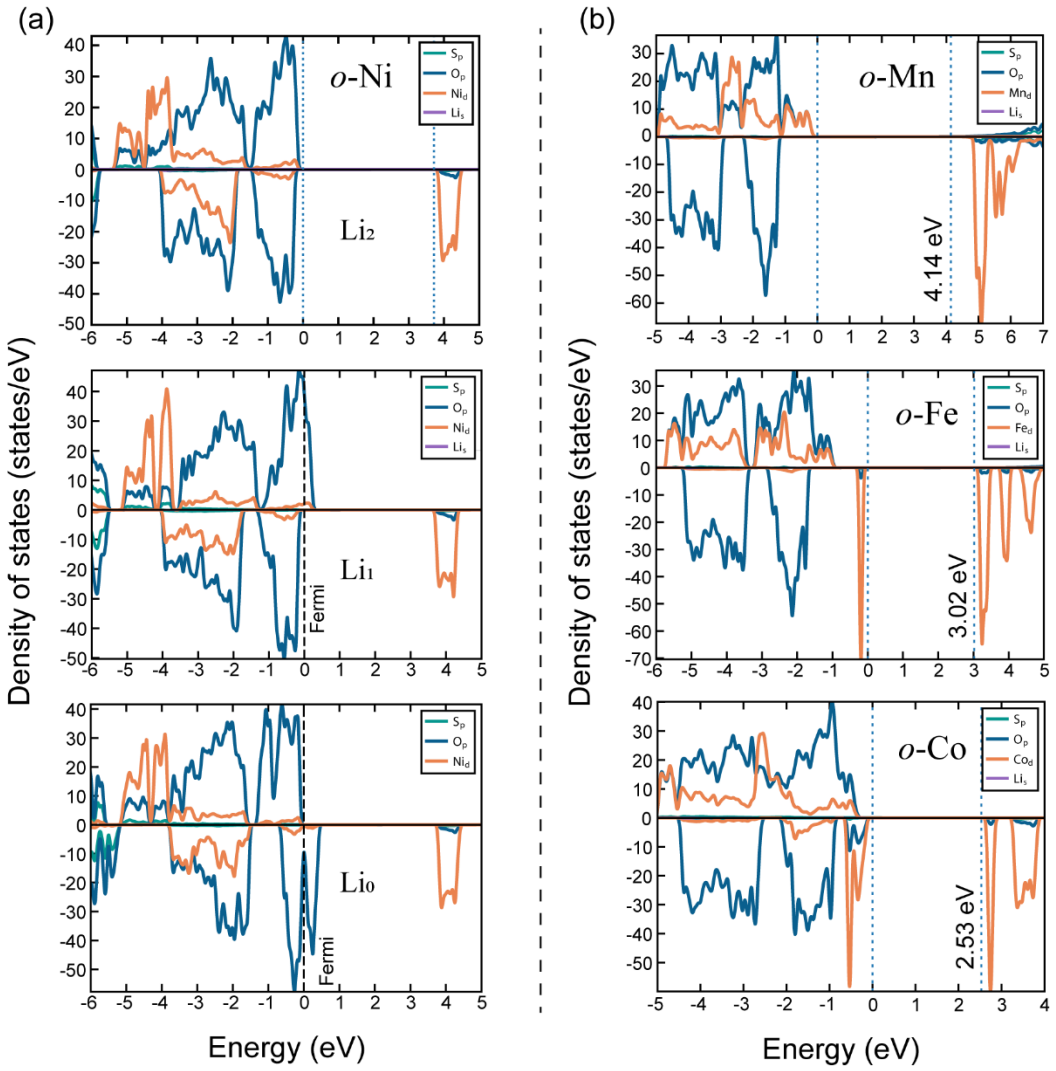

Figure S8. GGA+*U*-calculated pDOS of (a) o-$Li_xNi(SO_4)_2$ and (b) o-$Li_2M(SO_4)_2$, where M = Mn (top panel), Fe (middle), and Co (bottom). In (a), the top, middle, and bottom panels represent different levels of (de)lithiation, namely, x = 2, 1, and 0, respectively. Notations on each panel are identical to **Figure S3.**

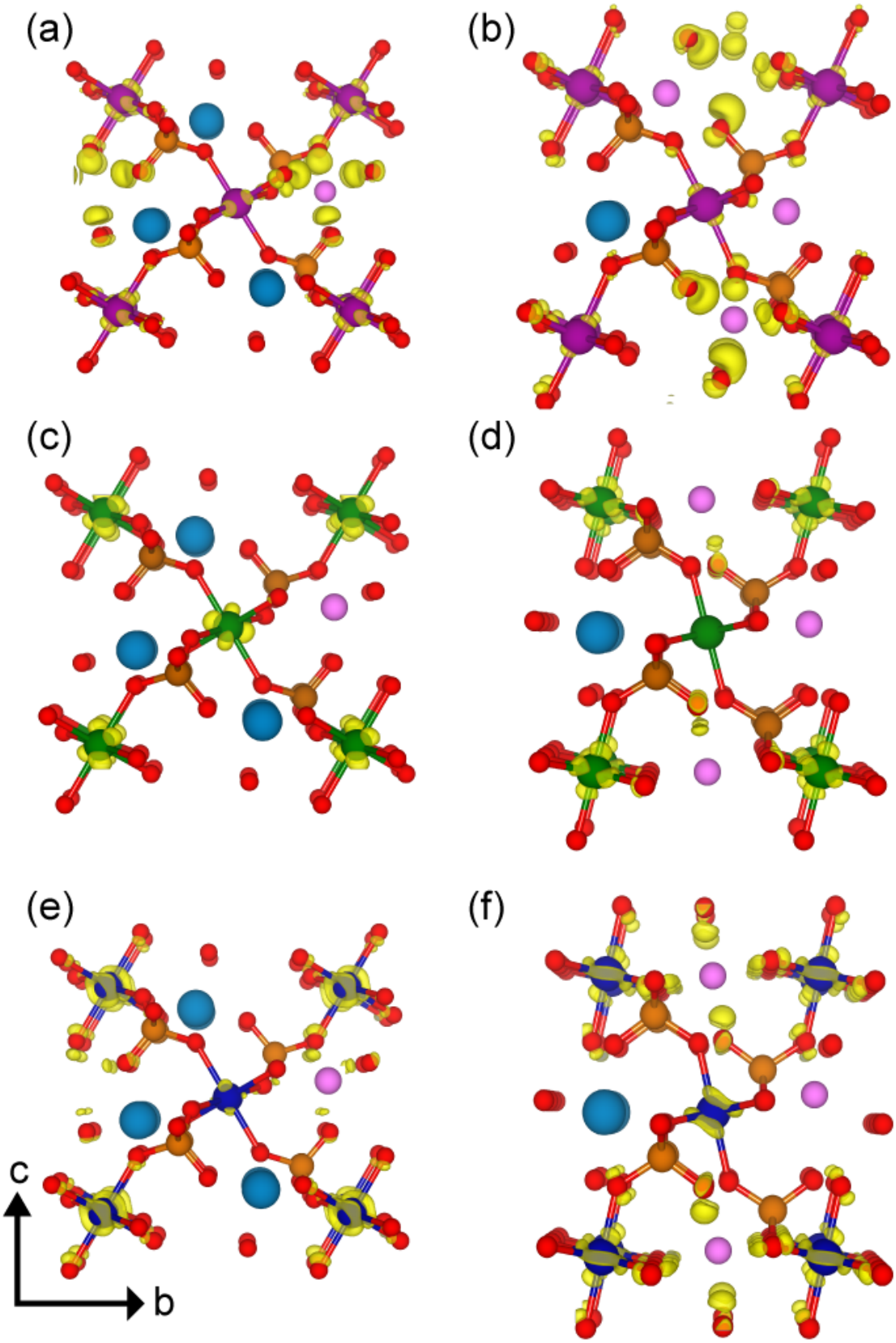

Figure S9. Electron density difference for Li-removal in (a) $Li_2Mn(SO_4)_2$, (b) $LiMn(SO_4)_2$, (c) $Li_2Fe(SO_4)_2$, (d) $LiFe(SO_4)_2$, (e) $Li_2Co(SO_4)_2$, and (f) $LiCo(SO_4)_2$. Red, blue, orange, purple, green, dark blue, and pink spheres represent O, Li, S, Mn, Fe, Co, and Li-vacancy, respectively. Isosurfaces are at 0.008 (Mn), 0.02 (Fe), and 0.015 $e^-/bohr^3$ (Co).

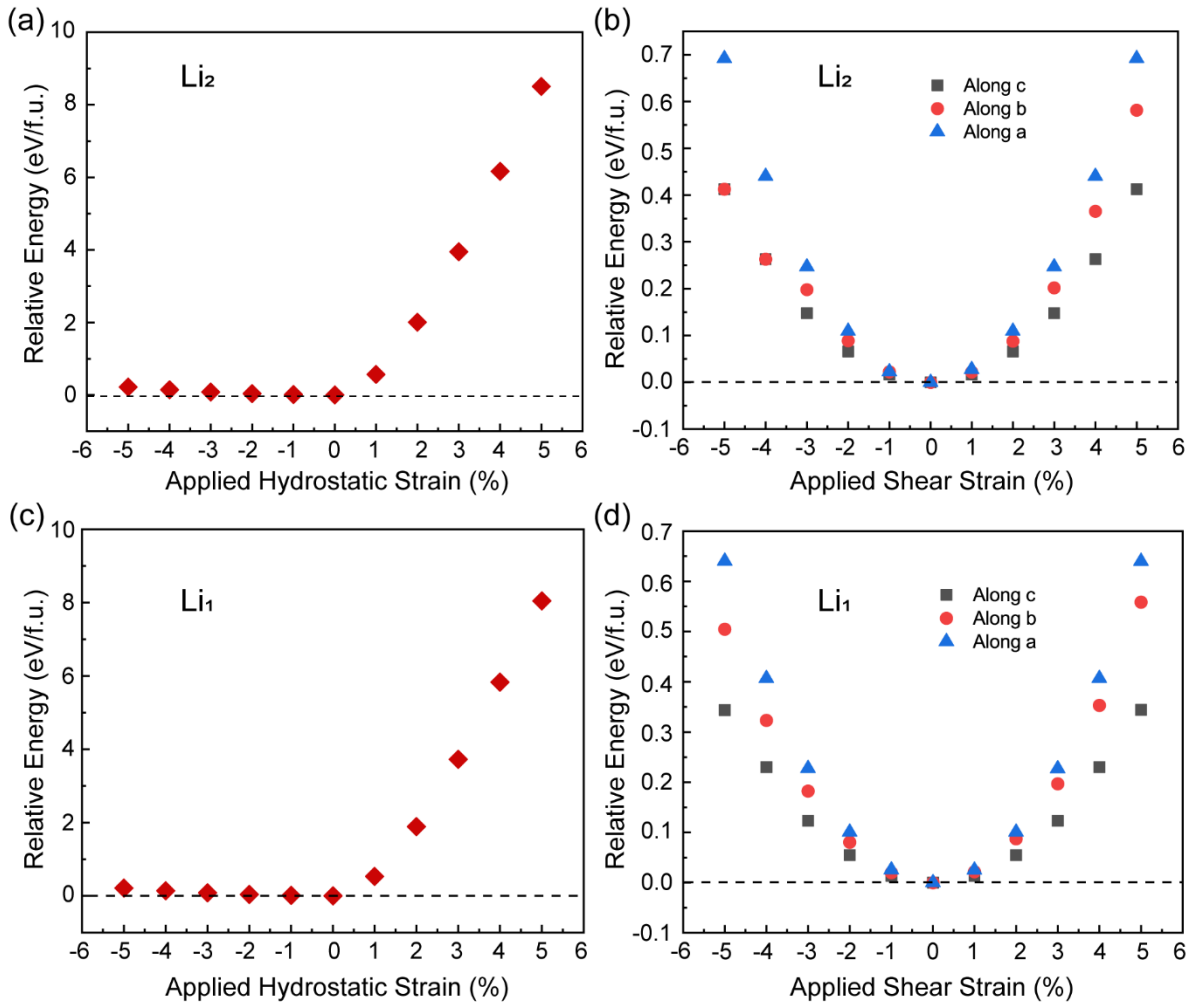

Figure S10. SCAN+*U* calculated energy, relative to the ground state configuration (in eV/f.u.), as a function of applied hydrostatic strain (panels a and c) and applied shear strain (b and d) in m-$Li_2Ni(SO_4)_2$ (a and b) and $LiNi(SO_4)_2$ (c and d). Applied strain in both panels are given in %, relative to the ground state configuration. Black squares, red circles, and blue triangles in the right panel indicate shear strains applied along the *c*, *b*, and *a*-axis of the monoclinic unit cell.

Table S1. Optimized lattice parameters of o-$Li_2Ni(SO_4)_2$ (M=Mn, Fe, Co, and Ni) estimated using SCAN+*U* and GGA+*U* approximations, compared with experimental values.

System		a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	V(Å^3)
$Li_2Mn(SO_4)_2$	GGA+*U*	9.51971	9.39573	14.03362	90.00	90.00	90.00	1255.23138
	SCAN+*U*	9.34368	9.24819	13.73874	90.00	90.00	90.00	1187.19290
$Li_2Fe(SO_4)_2$	GGA+*U*	9.38245	9.31127	13.86869	89.9999	90.0002	89.9999	1211.60352
	SCAN+*U*	9.18221	9.17010	13.61174	90.0001	90.0003	90.00	1146.13246
	Expt.	9.27980	9.20890	13.67650	90.00	90.00	90.00	1168.74938
$Li_2Co(SO_4)_2$	GGA+*U*	9.31610	9.20287	13.82582	90.00	90.00	90.00	118535436
	SCAN+*U*	9.16169	9.04557	13.57579	89.9996	90.00	89.998	1125.06175
	Expt.	9.20688	9.10175	13.71190	90.00	90.00	90.00	1149.03965
$Li_2Ni(SO_4)_2$	GGA+*U*	9.24625	9.13135	13.70520	90.00	90.00	90.00	1157.13982
	SCAN+*U*	9.09432	8.97466	13.45300	90.0001	90.00	90.00	1098.01195
	Expt.	9.12600	9.00100	13.54300	90.00	90.00	90.00	1112.46447

Table S2. Calculated and experimental average bond length, Baur's distortion index and bond angle variance of SO_4 and MO_6 polyhedra of m-$Li_2M(SO_4)_2$ (M=Mn, Fe, Co, and Ni).

System		**Bond-type**	**Average Bond Length (Å)**	**Distortion Index**	**Bond angle variance (°^{2})**
$Li_2Mn(SO_4)_2$	GGA+*U*	Mn-O	2.2124	0.02098	40.3915
		S-O	1.4898	0.00408	3.2049
	SCAN+*U*	Mn-O	2.1750	0.01686	40.4581
		S-O	1.4713	0.00420	3.1805
	Expt.	Mn-O	2.2029	0.01588	42.2134
		S-O	1.4566	0.00543	4.3430
$Li_2Fe(SO_4)_2$	GGA+*U*	Fe-O	2.1625	0.01649	32.8736
		S-O	1.4902	0.00525	4.2667
	SCAN+*U*	Fe-O	2.1290	0.01342	31.8448
		S-O	1.4717	0.00529	3.9191
	Expt.	Fe-O	2.1036	0.01179	39.7825
		S-O	1.4899	0.04329	28.2719
$Li_2Co(SO_4)_2$	GGA+*U*	Co-O	2.1351	0.01336	33.2996
		S-O	1.4898	0.00624	4.0917
	SCAN+*U*	Co-O	2.1036	0.01024	33.5848
		S-O	1.4710	0.00612	3.6361
	Expt.	Co-O	2.1100	0.00811	35.1295
		S-O	1.4773	0.00776	3.1783
$Li_2Ni(SO_4)_2$	GGA+*U*	Ni-O	2.1099	0.01630	29.5633
		S-O	1.4886	0.00659	4.2634
	SCAN+*U*	Ni-O	2.0738	0.01266	27.5136
		S-O	1.4707	0.00686	3.7888
	Expt.	Ni-O	2.1776	0.02216	28.0094
		S-O	1.4814	0.01109	46.9046

Table S3. Calculated and experimental average bond length, Baur's distortion index and bond angle variance of SO_4 and MO_6 polyhedra of o-$Li_2M(SO_4)_2$ (M=Mn, Fe, Co, and Ni).

System		Bond-type	Average Bond Length (Å)	Distortion Index	Bond angle variance (^{o2})
$Li_2Mn(SO_4)_2$	GGA+*U*	Mn-O	2.2010	0.02046	20.2946
		S-O	1.4914	0.00369	11.2927
	SCAN+*U*	Mn-O	2.1596	0.01774	20.7383
		S-O	1.4742	0.00457	11.0910
$Li_2Fe(SO_4)_2$	GGA+*U*	Fe-O	2.1511	0.01364	20.2515
		S-O	1.4912	0.00294	11.5389
	SCAN+*U*	Fe-O	2.1120	0.00973	23.3890
		S-O	1.4746	0.00502	12.7614
	Expt.	Fe-O	2.1323	0.01657	24.4085
		S-O	1.4929	0.00083	17.2093
$Li_2Co(SO_4)_2$	GGA+*U*	Co-O	2.1213	0.01813	18.03303
		S-O	1.4932	0.00592	23.0551
	SCAN+*U*	Co-O	2.0858	0.01697	18.4334
		S-O	1.4722	0.00226	12.2298
	Expt.	Co-O	2.0861	0.01286	17.1494
		S-O	1.4831	0.01379	12.1005
$Li_2Ni(SO_4)_2$	GGA+*U*	Ni-O	2.0922	0.01518	15.3757
		S-O	1.4927	0.00613	15.3757
	SCAN+*U*	Ni-O	2.0534	0.01051	15.8152
		S-O	1.4745	0.00624	14.2162
	Expt.	Ni-O	2.0584	0.01314	15.6537
		S-O	1.4736	0.00563	13.0296

Table S4. SCAN+*U* predicted on-site, averaged, magnetic moments of transition elements and corresponding electronic configurations.

System	Magnetic Moment	Corresponding Electronic configuration
$Li_2Mn(SO_4)_2$	4.657	$t_{2g}^3 e_g^2$
$LiMn(SO_4)_2$	3.889	$t_{2g}^3 e_g^1$
$Mn(SO_4)_2$	3.033	$t_{2g}^3 e_g^0$
$Li_2Fe(SO_4)_2$	3.745	$t_{2g}^4 e_g^2$
$LiFe(SO_4)_2$	4.361	$t_{2g}^3 e_g^2$
$Fe(SO_4)_2$	4.301	$t_{2g}^3 e_g^2$
$Li_2Co(SO_4)_2$	2.802	$t_{2g}^5 e_g^2$
$LiCo(SO_4)_2$	3.224	$t_{2g}^4 e_g^2$
$Co(SO_4)_2$	3.236	$t_{2g}^4 e_g^2$
$Li_2Ni(SO_4)_2$	1.785	$t_{2g}^6 e_g^2$
$LiNi(SO_4)_2$	1.857	$t_{2g}^6 e_g^2$
$Ni(SO_4)_2$	1.831	$t_{2g}^6 e_g^2$

Table S5. SCAN+*U* predicted change in on-site magnetic moment of individual oxygen ions at various (de)lithiation states of $Li_xNi(SO_4)_2$.

	$Li_2Ni(SO_4)_2$	**$LiNi(SO_4)_2$**	**$Ni(SO_4)_2$**
O1	-0.001	0.053	**0.520**
O2	-0.001	**0.324**	**0.519**
O3	-0.001	0.053	**0.520**
O4	-0.001	**0.323**	**0.519**
O5	0.030	0.051	0.073
O6	0.029	0.078	0.075
O7	0.029	0.051	0.073
O8	0.030	0.078	0.074
O9	0.026	0.038	0.060
O10	0.025	0.061	0.059
O11	0.025	0.038	0.060
O12	0.026	0.061	0.060
O13	0.029	0.064	**0.314**
O14	0.029	**0.349**	**0.314**
O15	0.029	0.063	**0.314**
O16	0.029	**0.349**	**0.314**

Table S6. SCAN+*U* predicted change in on-site magnetic moment of individual oxygen ions at various (de)lithiation states of $Li_xMn(SO_4)_2$.

	$Li_2Mn(SO_4)_2$	**$LiMn(SO_4)_2$**	**$Mn(SO_4)_2$**
O1	0	0.001	0.009
O2	0	0.001	0.008
O3	0	0.001	0.009
O4	0	0.001	0.008
O5	0.018	0.011	-0.023
O6	0.018	0.015	-0.025
O7	0.018	0.011	-0.023
O8	0.018	0.015	-0.024
O9	0.017	-0.003	-0.015
O10	0.017	-0.005	-0.016
O11	0.017	-0.003	-0.015
O12	0.017	-0.005	-0.016
O13	0.017	-0.021	-0.024
O14	0.017	-0.035	-0.026
O15	0.017	-0.021	-0.024
O16	0.017	-0.034	-0.025

Table S7. SCAN+*U* predicted change in on-site magnetic moment of individual oxygen ions at various (de)lithiation states of $Li_xCo(SO_4)_2$.

	$Li_2Co(SO_4)_2$	**$LiCo(SO_4)_2$**	**$Co(SO_4)_2$**
O1	0	0.009	0.276
O2	0	0.020	0.22
O3	0	0.009	0.22
O4	0	0.020	0.276
O5	0.025	0.081	0.154
O6	0.025	0.102	0.176
O7	0.025	0.081	0.176
O8	0.025	0.102	0.154
O9	0.020	0.068	0.185
O10	0.019	0.11	0.176
O11	0.019	0.068	0.176
O12	0.020	0.11	0.185
O13	0.023	0.099	0.192
O14	0.023	0.184	0.199
O15	0.023	0.099	0.199
O16	0.023	0.184	0.192

Table S8. SCAN+*U* predicted change in on-site magnetic moment of individual oxygen ions at various (de)lithiation states of $Li_xFe(SO_4)_2$.

	$Li_2Fe(SO_4)_2$	**$LiFe(SO_4)_2$**	**$Fe(SO_4)_2$**
O1	0	0.006	-0.180
O2	0	0.006	-0.185
O3	0	0.006	-0.180
O4	0	0.007	-0.184
O5	0.021	0.086	0.006
O6	0.021	0.085	0.003
O7	0.021	0.085	0.006
O8	0.021	0.086	0.002
O9	0.020	0.078	0.003
O10	0.020	0.078	-0.004
O11	0.020	0.078	0.003
O12	0.020	0.079	-0.004
O13	0.024	0.075	-0.005
O14	0.024	0.081	-0.003
O15	0.024	0.076	-0.005
O16	0.024	0.081	-0.003

Table S9. (a) Mulliken and (b) Löwdin charge populations at various (de)lithiation states of m-$Li_xNi(SO_4)_2$, calculated using LOBSTER package, based on SCAN+*U*-computed charge densities.

(a)

Element	$Li_2Ni(SO_4)_2$	$LiNi(SO_4)_2$	$Ni(SO_4)_2$
Ni1	1.51	1.58	1.60
Ni2	1.51	1.58	1.60
O1	-1.14	-1.06	-0.67
O2	-1.14	-0.87	-0.67
O3	-1.14	-1.06	-0.67
O4	-1.14	-0.87	-0.67
O5	-1.08	-1.07	-1.03
O6	-1.08	-1.02	-1.03
O7	-1.08	-1.07	-1.03
O8	-1.08	-1.02	-1.03
O9	-1.11	-1.11	-1.06
O10	-1.11	-1.05	-1.06
O11	-1.11	-1.11	-1.06
O12	-1.11	-1.05	-1.06
O13	-1.10	-1.09	-0.91
O14	-1.10	-0.86	-0.90
O15	-1.10	-1.09	-0.91
O16	-1.10	-0.86	-0.90

(b)

Element	$Li_2Ni(SO_4)_2$	$LiNi(SO_4)_2$	$Ni(SO_4)_2$
Ni1	1.39	1.44	1.42
Ni2	1.39	1.44	1.42
O1	-1.03	-0.97	-0.62
O2	-1.03	-0.78	-0.62
O3	-1.03	-0.97	-0.62
O4	-1.03	-0.78	-0.62
O5	-1.00	-0.99	-0.94
O6	-1.00	-0.93	-0.95
O7	-1.00	-0.99	-0.94
O8	-1.00	-0.93	-0.95
O9	-1.02	-1.02	-0.97
O10	-1.02	-0.96	-0.97
O11	-1.02	-1.02	-0.97
O12	-1.02	-0.96	-0.97
O13	-1.01	-1.00	-0.83
O14	-1.01	-0.78	-0.83
O15	-1.01	-1.00	-0.83
O16	-1.01	-0.78	-0.83

Table S10. Mulliken charge population at various (de)lithiation states of m-$Li_xMn(SO_4)_2$ calculated using LOBSTER package, based on SCAN+*U*-computed charge densities.

Element	$Li_2Mn(SO_4)_2$	$LiMn(SO_4)_2$	$Mn(SO_4)_2$
Mn1	1.61	1.92	2.05
Mn2	1.61	1.92	2.05
O1	-1.14	-1.07	-0.97
O2	-1.14	-1.07	-0.97
O3	-1.14	-1.07	-0.97
O4	-1.14	-1.07	-0.97
O5	-1.10	-1.06	-0.95
O6	-1.10	-1.05	-0.94
O7	-1.10	-1.06	-0.95
O8	-1.10	-1.05	-0.94
O9	-1.11	-1.08	-0.96
O10	-1.11	-1.03	-0.97
O11	-1.11	-1.08	-0.96
O12	-1.11	-1.03	-0.97
O13	-1.10	-1.05	-0.94
O14	-1.10	-0.99	-0.94
O15	-1.10	-0.105	-0.94
O16	-1.10	-0.99	-0.94

Table S11. Mulliken charge population at various (de)lithiation states states of m-$Li_xFe(SO_4)_2$ calculated using LOBSTER package, based on SCAN+*U*-computed charge densities.

Element	$Li_2Fe(SO_4)_2$	$LiFe(SO_4)_2$	$Fe(SO_4)_2$
Fe1	1.58	2.09	2.14
Fe2	1.58	2.09	2.14
O1	-1.14	-1.08	-0.89
O2	-1.14	-1.08	-0.88
O3	-1.14	-1.08	-0.89
O4	-1.14	-1.08	-0.88
O5	-1.09	-1.06	-1.01
O6	-1.09	-1.06	-1.01
O7	-1.09	-1.06	-1.01
O8	-1.09	-1.06	-1.01
O9	-1.11	-1.08	-1.02
O10	-1.11	-1.07	-1.02
O11	-1.11	-1.08	-1.02
O12	-1.11	-1.07	-1.02
O13	-1.11	-1.07	-1.01
O14	-1.11	-1.08	-1.01
O15	-1.11	-1.07	-1.01
O16	-1.11	-1.08	-1.01

Table S12. Mulliken charge population at various (de)lithiation states of m-$Li_2Co(SO_4)_2$ calculated using LOBSTER package, based on SCAN+*U*-computed charge densities.

Element	$Li_2Co(SO_4)_2$	$LiCo(SO_4)_2$	$Co(SO_4)_2$
Co1	1.57	1.90	1.97
Co2	1.57	1.90	1.97
O1	-1.14	-1.07	-0.76
O2	-1.14	-1.07	-0.80
O3	-1.14	-1.07	-0.80
O4	-1.14	-1.07	-0.76
O5	-1.09	-1.02	-0.92
O6	-1.09	-1.02	-0.91
O7	-1.09	-1.02	-0.91
O8	-1.09	-1.02	-0.92
O9	-1.11	-1.05	-0.92
O10	-1.11	-1.05	-0.93
O11	-1.11	-1.05	-0.93
O12	-1.11	-1.05	-0.92
O13	-1.11	-1.05	-0.90
O14	-1.11	-1.05	-0.90
O15	-1.11	-1.05	-0.90
O16	-1.11	-1.05	-0.90

Table S13. SCAN+*U*-calculated S-O and M-O bond lengths at various (de)lithiation states for m-$Li_xM(SO_4)_2$ (M = Ni, Mn, Fe and Co).

$Li_2Ni(SO_4)_2$	$LiNi(SO_4)_2$	$Ni(SO_4)_2$
(Ni1-O6) = 2.12365 Å	(Ni1-O6) = 2.11576 Å	(Ni1-O6) = 2.03590 Å
(Ni1-O11) = 2.03924 Å	(Ni1-O11) = 2.05477 Å	(Ni1-O11) = 2.03518 Å
(Ni1-O16) = 2.06790 Å	(Ni1-O16) = 1.99274 Å	(Ni1-O16) = 2.02626 Å
(Ni1-O15) = 2.07702 Å	(Ni1-O15) = 2.04683 Å	(Ni1-O15) = 2.03603 Å
(Ni1-O12) = 2.03538 Å	(Ni1-O12) = 2.03403 Å	(Ni1-O12) = 2.03341 Å
(Ni1-O5) = 2.09935 Å	(Ni1-O5) = 2.04563 Å	(Ni1-O5) = 2.03062 Å
(Ni2-O13) = 2.06790 Å	(Ni2-O13) = 2.04667 Å	(Ni2-O13) = 2.03546 Å
(Ni2-O7) = 2.12364 Å	(Ni2-O7) = 2.04545 Å	(Ni2-O7) = 2.03094 Å
(Ni2-O10) = 2.03922 Å	(Ni2-O10) = 2.03440 Å	(Ni2-O10) = 2.03375 Å
(Ni2-O9) = 2.03538 Å	(Ni2-O9) = 2.05459 Å	(Ni2-O9) = 2.03502 Å
(Ni2-O8) = 2.09936 Å	(Ni2-O8) = 2.11490 Å	(Ni2-O8) = 2.03557 Å
(Ni2-O14) = 2.07705 Å	(Ni2-O14) = 1.99412 Å	(Ni2-O14) = 2.02644 Å

$Li_2Ni(SO_4)_2$	$LiNi(SO_4)_2$	$Ni(SO_4)_2$
(S1-O5) = 1.48130(0) Å	(S1-O5) = 1.48377 Å	(S1-O5) = 1.44933 Å
(S1-O1) = 1.44990(0) Å	(S1-O1) = 1.43421 Å	(S1-O1) = 1.49229 Å
(S1-O9) = 1.47531(0) Å	(S1-O9) = 1.48185 Å	(S1-O9) = 1.44386 Å
(S1-O13) = 1.47506(0) Å	(S1-O13)= 1.48163 Å	(S1-O13) = 1.48141 Å
(S2-O14) = 1.47518(0) Å	(S2-O14) = 1.50160 Å	(S2-O14)= 1.48176 Å
(S2-O10) = 1.47631(0) Å	(S2-O10) = 1.44639 Å	(S2-O10)= 1.44401 Å
(S2-O2) = 1.45054(0) Å	(S2-O2) = 1.47039 Å	(S2-O2) = 1.49205 Å
(S2-O6) = 1.48086(0) Å	(S2-O6) = 1.45015 Å	(S2-O6) = 1.44891 Å
(S3-O15) = 1.47518(0) Å	(S3-O15) = 1.48162 Å	(S3-O15)= 1.48140 Å
(S3-O7) = 1.48086(0) Å	(S3-O7) = 1.48372 Å	(S3-O7) = 1.44932 Å
(S3-O11) = 1.47630(0) Å	(S3-O11) = 1.48187 Å	(S3-O11)= 1.44394 Å
(S3-O3) = 1.45054(0) Å	(S3-O3) = 1.43413 Å	(S3-O3) = 1.49232 Å
(S4-O4) = 1.44992(0) Å	(S4-O4) = 1.47011 Å	(S4-O4) = 1.49202 Å
(S4-O12) = 1.47530(0) Å	(S4-O12) = 1.44643 Å	(S4-O12) = 1.44413 Å
(S4-O8) = 1.48129(0) Å	(S4-O8) = 1.45027 Å	(S4-O8) = 1.44879 Å
(S4-O16) = 1.47503(0) Å	(S4-O16) = 1.50196 Å	(S4-O16) = 1.48170 Å

$Li_2Mn(SO_4)_2$	$LiMn(SO_4)_2$	$Mn(SO_4)_2$
(Mn1-O6) = 2.18736 Å	(Mn1-O6) = 2.17687 Å	(Mn1-O6) = 1.91301 Å
(Mn1-O11) = 2.12220 Å	(Mn1-O11) = 1.97186 Å	(Mn1-O11) = 1.90916 Å
(Mn1-O16) = 2.22025 Å	(Mn1-O16) = 1.90674 Å	(Mn1-O16) = 1.90003 Å
(Mn1-O15) = 2.22014 Å	(Mn1-O15) = 1.98723 Å	(Mn1-O15) = 1.90020 Å
(Mn1-O12) = 2.12210 Å	(Mn1-O12) = 1.92036 Å	(Mn1-O12) = 1.91823 Å
(Mn1-O5) = 2.18763 Å	(Mn1-O5) = 2.30486 Å	(Mn1-O5) = 1.91517 Å
(Mn2-O13) = 2.22025 Å	(Mn2-O13) = 1.98704 Å	(Mn2-O13) = 1.89995 Å
(Mn2-O7) = 2.18736 Å	(Mn2-O7) = 2.30458 Å	(Mn2-O7) = 1.91544 Å
(Mn2-O10) = 2.12220 Å	(Mn2-O10) = 1.92135 Å	(Mn2-O10) = 1.91799 Å
(Mn2-O9) = 2.12210 Å	(Mn2-O9) = 1.97243 Å	(Mn2-O9) = 1.90963 Å
(Mn2-O8) = 2.18765 Å	(Mn2-O8) = 2.17668 Å	(Mn2-O8) = 1.91274 Å
(Mn2-O14) = 2.22014 Å	(Mn2-O14) = 1.90618 Å	(Mn2-O14) = 1.90043 Å

$Li_2Mn(SO_4)_2$	$LiMn(SO_4)_2$	$Mn(SO_4)_2$
(S1-O5) = 1.48012 Å	(S1-O5) = 1.46125 Å	(S1-O5) = 1.49804 Å
(S1-O1) = 1.45904 Å	(S1-O1) = 1.41929 Å	(S1-O1) = 1.40121 Å
(S1-O9) = 1.47288 Å	(S1-O9) = 1.50712 Å	(S1-O9) = 1.50762 Å
(S1-O13) = 1.47374 Å	(S1-O13) = 1.50285 Å	(S1-O13) = 1.50113 Å
(S2-O14) = 1.47375 Å	(S2-O14) = 1.50770 Å	(S2-O14) = 1.50201 Å
(S2-O10) = 1.47285 Å	(S2-O10) = 1.49699 Å	(S2-O10) = 1.50613 Å
(S2-O2) = 1.45904 Å	(S2-O2) = 1.43209 Å	(S2-O2) = 1.40126 Å
(S2-O6) = 1.48013 Å	(S2-O6) = 1.45237 Å	(S2-O6) = 1.49914 Å
(S3-O15) = 1.47376 Å	(S3-O15) = 1.50279 Å	(S3-O15) = 1.50137 Å
(S3-O7) = 1.48015 Å	(S3-O7) = 1.46124 Å	(S3-O7) = 1.49814 Å
(S3-O11) = 1.47287 Å	(S3-O3) = 1.41928 Å	(S3-O11) = 1.50798 Å
(S3-O3) = 1.45897 Å	(S3-O11) = 1.50721 Å	(S3-O3) = 1.40121 Å
(S4-O4) = 1.45899 Å	(S4-O4) = 1.43213 Å	(S4-O4) = 1.40130 Å
(S4-O12) = 1.47290 Å	(S4-O12) = 1.49714 Å	(S4-O12) = 1.50599 Å
(S4-O8) = 1.48013 Å	(S4-O8) = 1.45236 Å	(S4-O8) = 1.49912 Å
(S4-O16) = 1.47375 Å	(S4-O16) = 1.50749 Å	(S4-O16) = 1.50203 Å

$Li_2Fe(SO_4)_2$	$LiFe(SO_4)_2$	$Fe(SO_4)_2$
(Fe1-O6) = 2.17040 Å	(Fe1-O6) = 1.99780 Å	(Fe1-O6) = 1.98399 Å
(Fe1-O11) = 2.10094 Å	l(Fe1-O11) = 2.03597 Å	(Fe1-O11) = 1.98263 Å
(Fe1-O16) = 2.11517 Å	l(Fe1-O16) = 2.02310 Å	(Fe1-O16) = 1.98201 Å
(Fe1-O15) = 2.11858 Å	l(Fe1-O15) = 2.04369 Å	(Fe1-O15) = 1.98580 Å
(Fe1-O12) = 2.09559 Å	l(Fe1-O12) = 2.03401 Å	(Fe1-O12) = 1.99253 Å
(Fe1-O5) = 2.17334 Å	l(Fe1-O5) = 1.98894 Å	(Fe1-O5) = 1.97956 Å
(Fe2-O13) = 2.11517 Å	(Fe2-O13) = 2.04524 Å	(Fe2-O13) = 1.98595 Å
(Fe2-O7) = 2.17054 Å	(Fe2-O7) = 1.99311 Å	(Fe2-O7) = 1.97946 Å
(Fe2-O10) = 2.10104 Å	(Fe2-O10) = 2.03242 Å	(Fe2-O10) = 1.99247 Å
(Fe2-O9) = 2.09559 Å	(Fe2-O9) = 2.03567 Å	(Fe2-O9) = 1.98282 Å
(Fe2-O8) = 2.17354 Å	(Fe2-O8) = 1.99551 Å	(Fe2-O8) = 1.98407 Å
(Fe2-O14) = 2.11824 Å	(Fe2-O14) = 2.02075 Å	(Fe2-O14) = 1.98197 Å

$Li_2Fe(SO_4)_2$	$LiFe(SO_4)_2$	$Fe(SO_4)_2$
(S1-O5) = 1.47663 Å	(S1-O5) = 1.47288 Å	l(S1-O5) = 1.47878 Å
(S1-O1) = 1.45590 Å	(S1-O9) = 1.49002 Å	l(S1-O9) = 1.48012 Å
(S1-O9) = 1.47299 Å	(S1-O1) = 1.42655 Å	l(S1-O1) = 1.43542 Å
(S1-O13) = 1.48077 Å	(S1-O13) = 1.49631 Å	l(S1-O13) = 1.47920 Å
(S2-O14) = 1.48077 Å	(S2-O14) = 1.49091 Å	(S2-O14) = 1.48023 Å
(S2-O10) = 1.47266 Å	(S2-O2) = 1.42697 Å	(S2-O2) = 1.43606 Å
(S2-O2) = 1.45608 Å	(S2-O10) = 1.49730 Å	(S2-O10) = 1.47905 Å
(S2-O6) = 1.47713 Å	(S2-O6) = 1.47106 Å	(S2-O6) = 1.47835 Å
(S3-O15) = 1.48071 Å	(S3-O15) = 1.49504 Å	(S3-O15) = 1.47921 Å
(S3-O7) = 1.47711 Å	(S3-O7) = 1.47206 Å	(S3-O7) = 1.47865 Å
(S3-O11) = 1.47266 Å	(S3-O11) = 1.49226 Å	(S3-O11) = 1.48008 Å
(S3-O3) = 1.45613 Å	(S3-O3) = 1.42691 Å	(S3-O3) = 1.43557 Å
(S4-O4) = 1.45597 Å	(S4-O4) = 1.42707 Å	(S4-O4) = 1.43588 Å
(S4-O12) = 1.47296 Å	(S4-O12) = 1.49524 Å	(S4-O12) = 1.47889 Å
(S4-O8) = 1.47658 Å	(S4-O8) = 1.47191 Å	(S4-O8) = 1.47850 Å
(S4-O16) = 1.48077 Å	(S4-O16) = 1.49293 Å	(S4-O16) = 1.48026 Å

$Li_2Co(SO_4)_2$	$LiCo(SO_4)_2$	$Co(SO_4)_2$
(Co1-O6) = 2.12335 Å	(Co1-O6) = 2.05906 Å	(Co1-O6) = 2.00399 Å
(Co1-O11) = 2.07338 Å	(Co1-O11) = 2.06748 Å	(Co1-O11) = 1.99577 Å
(Co1-O16) = 2.11503 Å	(Co1-O16) = 1.87982 Å	(Co1-O16) = 1.92431 Å
(Co1-O15) = 2.11641 Å	(Co1-O15) = 1.99580 Å	(Co1-O15) = 1.90834 Å
(Co1-O12) = 2.06921 Å	(Co1-O12) = 1.95123 Å	(Co1-O12) = 2.00657 Å
(Co1-O5) = 2.12421 Å	(Co1-O5) = 2.08089 Å	(Co1-O5) = 2.00595 Å
(Co2-O13) = 2.11504 Å	(Co2-O13) = 1.99526 Å	(Co2-O13) = 1.92429 Å
(Co2-O7) = 2.12335 Å	(Co2-O7) = 2.08059 Å	(Co2-O7) = 2.00396 Å
(Co2-O10) = 2.07339 Å	(Co2-O10) = 1.95141 Å	(Co2-O10) = 1.99584 Å
(Co2-O9) = 2.06921 Å	(Co2-O9) = 2.06788 Å	(Co2-O9) = 2.00661 Å
(Co2-O8) = 2.12420 Å	(Co2-O8) = 2.05876 Å	(Co2-O8) = 2.00599 Å
(Co2-O14) = 2.11642 Å	(Co2-O14) = 1.87980 Å	(Co2-O14) = 1.90832 Å

$Li_2Co(SO_4)_2$	$LiCo(SO_4)_2$	$Co(SO_4)_2$
(S1-O5) = 1.48201 Å	(S1-O5) = 1.47676(0) Å	(S1-O5) = 1.46576 Å
(S1-O1) = 1.45300 Å	(S1-O1) = 1.41797(0) Å	(S1-O9) = 1.47448 Å
(S1-O9) = 1.47362 Å	(S1-O9) = 1.49453(0) Å	(S1-O1) = 1.44833 Å
(S1-O13) = 1.47535 Å	(S1-O13) = 1.49647(0) Å	(S1-O13) = 1.48578 Å
(S2-O14) = 1.47538 Å	(S2-O14) = 1.50678(0) Å	(S2-O14) = 1.49110 Å
(S2-O10) = 1.47350 Å	(S2-O2) = 1.43067(0) Å	(S2-O2) = 1.43831 Å
(S2-O2) = 1.45310 Å	(S2-O6) = 1.46841(0) Å	(S2-O10) = 1.47569 Å
(S2-O6) = 1.48221 Å	(S2-O10) = 1.47793(0) Å	(S2-O6) = 1.47211 Å
(S3-O15) = 1.47538 Å	(S3-O15) = 1.49652(0) Å	(S3-O15) = 1.49121 Å
(S3-O7) = 1.48221 Å	(S3-O7) = 1.47681(0) Å	(S3-O7) = 1.47211 Å
(S3-O11) = 1.47350 Å	(S3-O11) = 1.49461(0) Å	(S3-O11) = 1.47585 Å
(S3-O3) = 1.45310 Å	(S3-O3) = 1.41794(0) Å	(S3-O3) = 1.43838 Å
(S4-O4) = 1.45301 Å	(S4-O4) = 1.43063(0) Å	(S4-O4) = 1.44849 Å
(S4-O12) = 1.47361 Å	(S4-O12) = 1.47802(0) Å	(S4-O12) = 1.47458 Å
(S4-O8) = 1.48202 Å	(S4-O8) = 1.46844(0) Å	(S4-O8) = 1.46577 Å
(S4-O16) = 1.47535 Å	(S4-O16) = 1.50675(0) Å	(S4-O16) = 1.48560 Å