Supplementary Material (ESI) for Energy & Environmental Science

Supplemental document

Thermodynamic analysis on energy densities of batteries

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Supplementary data caption:

Table S1. All chemical reactions calculated.

Table S2. Thermodynamic data of typical battery systems. The volumetric energy densities of the batteries containing gas components are not calculated.

Table S3. Thermodynamic data of selected typical lithium battery systems.

Table S4. Thermodynamic data of all lithium battery systems calculated.

Table S5. Thermodynamic data of lithium-ion battery systems with high gravimetric energy densities.

Table S6. Capacity values of typical lithium-free cathodes.

Table S7. Capacity values of lithium-contained cathodes.

Table S8. Capacity values of typical anodes.

Table S9. Capacity values calculated in all.

Table S10. Calculated EMF values (V) of conversion reactions between binary transition mental compounds and lithium.

Table S11. Calculated EMF (V) of conversion reactions between fluorides and

Table S1. All chemical reactions calculated.

Li						
M_aX_b	n	Δ_rG (kJ mol^{-1})	EMF (V)	Capacity (m A h g^{-1})	Cal. Energy density (W h kg^{-1})	Cal. Energy density (W h L^{-1})
F						
BeF_2	2.00	-196.0	1.016	1140.3	894.1	1125.3
NaF	1.00	-41.4	0.429	638.3	235.0	409.2
MgF_2	2.00	-104.3	0.540	860.4	380.3	632.8
AlF_3	3.00	-332.0	1.147	957.5	880.0	1395.5
KF	1.00	-49.9	0.517	461.3	213.1	380.5
CaF_2	2.00	0.2	-0.001	686.6	-0.6	-1.1
ScF_3	3.00	-223.3	0.771	788.7	505.1	775.8
TiF_3	3.00	-401.1	1.386	766.8	886.5	1501.9
TiF_4	4.00	-791.8	2.052	865.5	1450.6	2284.9
VF_3	3.00	-536.4	1.853	744.9	1157.3	2096.1
CrF_3	3.00	-659.7	2.279	737.7	1411.5	2707.6
MnF_2	2.00	-368.3	1.909	576.8	957.8	2073.2
MnF_3	3.00	-763.3	2.637	718.3	1597.1	3002.6
FeF_2	2.00	-506.8	2.626	571.2	1306.8	2876.5
FeF_3	3.00	-791.1	2.733	712.5	1644.1	3224.4
CoF_2	2.00	-528.2	2.737	553.0	1324.1	3074.0
CoF_3	3.00	-1044.1	3.607	693.6	2120.8	4211.1
NiF_2	2.00	-571.3	2.961	554.4	1435.2	3407.8
CuF	1.00	-327.7	3.396	324.7	1017.2	3696.7
CuF_2	2.00	-683.4	3.541	527.9	1644.7	3796.5
ZnF_2	2.00	-462.1	2.395	518.5	1094.6	2725.5
GaF_3	3.00	-677.8	2.342	634.5	1276.1	2795.8
RbF	1.00	-59.2	0.613	256.6	147.5	388.0
YF_3	3.00	-118.4	0.409	551.1	197.3	435.8
ZrF_2	2.00	-262.4	1.360	414.8	509.3	-
ZrF_3	3.00	-437.5	1.512	542.5	719.0	1647.2
ZrF_4	4.00	-540.9	1.402	641.1	770.6	1674.3

NbF_5	5.00	-1239.5	2.569	713.2	1546.7	2558.3
RuF_3	3.00	-	-	508.7	-	-
RuF_5	5.00	-2157.2	4.472	683.5	2596.7	5198.8
AgF	1.00	-400.7	4.153	211.3	831.8	3209.8
SnF_2	2.00	-573.9	2.974	342.1	934.6	2644.5
LaF_3	3.00	-139.3	0.481	410.4	178.6	536.0
CeF_3	3.00	-207.1	0.715	407.9	264.0	810.2
O						
BeO-α	2.00	18.9	-0.098	2143.1	-135.0	-153.0
B_2O_3	3.00	-244.7	0.845	2309.7	1221.5	1290.9
Na_2O	1.00	-92.9	0.962	864.9	680.0	967.8
MgO microcrystal	2.00	8.1	-0.042	1329.9	-41.5	-61.0
Al_2O_3	3.00	-50.7	0.175	1577.2	196.0	271.7
SiO_2 quartz	4.00	-266.1	0.689	1784.3	841.4	983.1
SiO_2 high cristobalite	4.00	-268.8	0.696	1784.3	850.0	960.5
P_4O_{10}	5.00	-722.2	1.497	1888.2	1898.3	2040.5
K_2O	1.00	-119.6	1.239	569.1	614.5	1005.1
CaO	2.00	42.1	-0.218	955.9	-167.2	-273.3
Sc_2O_3	3.00	67.9	-0.235	1166.0	-210.1	-331.8
TiO	2.00	-66.2	0.343	839.3	236.5	472.7
Ti_2O_3	3.00	-124.7	0.431	1118.8	373.7	629.6
Ti_3O_5	3.33	-162.9	0.506	1198.6	463.2	742.8
TiO_2-R	4.00	-233.3	0.605	1342.3	602.2	911.1
TiO_2	4.00	-233.6	0.605	1342.3	602.9	912.1
TiO_2-A	4.00	-239.5	0.621	1342.3	618.1	917.9
VO	2.00	-157.0	0.814	800.7	539.6	1259.5
V_2O_3	3.00	-272.2	0.940	1072.9	789.4	1390.1
VO_2	4.00	196.1	-0.508	1292.6	-492.0	-765.9
V_3O_5	3.33	-334.3	1.040	1151.2	921.8	-
V_2O_5	5.00	-693.3	1.437	1473.6	1532.6	2090.0
CrO_2	4.00	-577.5	1.496	1276.3	1435.4	2319.2
Cr_2O_3	3.00	-312.8	1.080	1058.0	897.3	1622.2
Cr_3O_4 (ΔH=-1513 kJ mol^{-1})	2.67	-237.9	0.925	974.7	719.7	1415.8

CrO_3	6.00	-1171.0	2.023	1608.2	2296.6	2828.0
MnO_2	4.00	-657.3	1.703	1233.1	1591.8	2642.1
Mn_2O_3	3.00	-401.3	1.386	1018.6	1117.3	2034.6
MnO	2.00	-198.3	1.028	755.6	649.4	1405.0
Mn_3O_4	2.67	-320.5	1.246	937.1	939.4	1765.9
FeO	2.00	-309.8	1.605	746.1	1003.8	2266.4
Fe_2O_3 hematite	3.00	-470.7	1.626	1007.0	1298.8	2412.2
Fe_3O_4 magnetite	2.67	-409.8	1.593	926.1	1189.6	2295.5
CoO	2.00	-347.0	1.798	715.3	1085.3	2561.4
Co_3O_4	2.67	-490.3	1.905	890.4	1378.7	2849.2
NiO	2.00	-349.5	1.811	717.6	1096.1	2695.1
Ni_2O_3	3.00	-	-	972.3	-	-
CuO	2.00	-431.5	2.236	673.9	1282.9	3105.0
Cu_2O	1.00	-207.6	2.152	374.6	734.7	2313.8
ZnO	2.00	-240.7	1.247	658.6	701.8	1649.7
Ga_2O_3	3.00	-342.7	1.184	857.9	830.9	1742.8
GeO	2.00	-324.0	1.679	604.7	877.9	-
GeO_2	4.00	-601.0	1.557	1024.5	1260.9	2179.1
As_4O_6 octahedral	3.00	-553.7	1.913	812.8	1284.4	2365.2
As_2O_5	5.00	-1011.9	2.097	1166.1	1878.5	3068.7
SeO_2	4.00	-950.9	2.464	966.2	1904.1	3298.4
Y_2O_3	3.00	66.5	-0.230	712.1	-138.2	-300.8
ZrO_2	4.00	-79.6	0.206	870.0	146.4	300.1
NbO	2.00	-169.3	0.877	492.2	382.9	1149.1
NbO_2	4.00	-381.9	0.990	858.3	694.9	1450.0
Nb_2O_5	5.00	-520.1	1.078	1008.3	862.0	1525.2
MoO_2	4.00	-589.4	1.527	837.9	1051.5	2281.3
MoO_3	6.00	-1015.6	1.754	1117.2	1520.1	2597.4
RuO_2	4.00	-842.4	2.183	805.6	1454.9	3301.9
RuO_4	8.00	-2092.6	2.711	1298.9	2635.0	3770.7
AgO	2.00	-575.0	2.980	432.7	1159.6	3757.3
Ag_2O	1.00	-275.0	2.850	231.3	622.0	2625.8
Ag_2O_3	3.00	-902.5	3.118	609.7	1641.9	-
La_2O_3	3.00	11.1	-0.038	493.6	-16.8	-48.2

CeO_2	4.00	-97.8	0.253	622.9	135.9	358.2
Ce_2O_3	3.00	11.3	-0.039	489.9	-17.0	-47.9
WO_2	4.00	-588.5	1.525	496.7	671.1	2271.2
WO_3	6.00	-919.6	1.589	693.6	934.0	2318.3
Na_2O_2	1.00	-61.6	0.639	687.4	372.7	636.4
K_2O_2	1.00	-72.9	0.756	486.4	326.5	522.9
Ag_2O_2	1.00	-299.3	3.102	216.4	635.5	2804.1
NaO_2	1.00	-	-	487.4	-	-
KO_2	1.00	-	-	377.0	-	-
CaO_2	1.00	-	-	371.8	-	-
S						
BeS	2.00	-206.0	1.068	1304.9	1041.2	1318.4
B_2S_3	3.00	-534.7	1.847	1364.8	1862.8	2016.7
Na_2S	1.00	-44.6	0.462	686.8	269.5	364.1
MgS	2.00	-97.2	0.504	950.9	384.3	574.1
Al_2S_3	3.00	-338.5	1.169	1070.9	980.4	1234.6
SiS_2	4.00	-665.4	1.724	1162.5	1540.5	1901.6
P_4S_3	1.50	-289.5	2.000	730.6	1229.0	1725.6
P_4S_7	3.50	-693.5	2.054	1077.1	1729.4	2259.3
P_2S_5	5.00	-1027.9	2.131	1205.8	1957.7	2384.6
K_2S	1.00	-37.5	0.389	486.1	167.8	233.1
CaS	2.00	38.4	-0.199	743.0	-124.0	-198.1
Sc_2S_3	3.00	-	-	864.1	-	-
TiS_2	4.00	-475.8	1.233	957.2	945.7	1550.8
TiS	2.00	-168.9	0.875	670.6	500.2	1003.6
Ti_2S_3	3.00	-	-	837.8	-	-
VS	2.00	-	-	645.8	-	-
V_2S_3	3.00	-	-	811.8	-	-
VS_2	4.00	-	-	931.6	-	-
V_2S_5	5.00	-	-	1022.1	-	-
CrS	2.00	-264.6	1.371	637.7	750.3	-
Cr_2S_3	3.00	-574.6	1.985	803.3	1319.9	2435.0
MnS	2.00	-220.6	1.143	616.1	607.4	1210.5
MnS_2	4.00	-653.0	1.692	900.4	1235.4	-
FeS	2.00	-338.6	1.755	609.7	924.0	2104.1
$FeS_{2(marcasite}$	4.00	-721.9	1.870	893.6	1357.3	2642.3

)						
$FeS_{2(pyrite)}$	4.00	-711.1	1.843	893.6	1337.0	2602.7
CoS	2.00	-	-	589.0	-	-
Co_2S_3	3.00	-	-	751.2	-	-
CoS_2	4.00	-732.4	1.898	871.1	1348.7	2523.6
Co_3S_4	2.67	-423.0	1.644	702.8	977.6	-
NiS	2.00	-359.5	1.863	590.6	954.3	2349.8
Ni_3S_4	2.67	-488.0	1.897	704.5	1130.1	2423.8
Ni_3S_2	1.33	-222.7	1.731	446.3	692.4	-
NiS_2	4.00	-753.3	1.952	872.8	1389.5	-
CuS	2.00	-385.4	1.997	560.6	977.7	2323.1
Cu_2S	1.00	-176.4	1.828	336.8	566.3	1800.9
ZnS	2.00	-237.7	1.232	550.0	593.0	1321.3
Ga_2S_3	3.00	-405.6	1.401	682.4	812.7	1590.7
GaS	2.00	-234.3	1.214	526.6	562.7	1242.9
GeS	2.00	-367.5	1.904	511.9	860.8	1980.9
GeS_2	4.00	-723.4	1.874	783.8	1221.3	2062.4
As_2S_3	3.00	-574.2	1.984	653.6	1108.8	2139.5
Se_2S_6	6.00	-	-	918.1	-	-
Se_4S_4	2.00	-	-	482.8	-	-
RuS_2	4.00	-	-	648.9	-	-
Y_2S_3	3.00	-	-	586.9	-	-
ZrS_2	4.00	-308.0	0.798	690.1	467.2	928.5
NbS_2	4.00	-	-	690.1	-	-
MoS_2	4.00	-652.1	1.690	669.7	964.3	2166.0
Mo_2S_3	3.00	-519.2	1.794	558.2	874.8	2276.0
Ag_2S(argentite)	1.00	-199.2	2.064	216.3	422.8	1835.8
LaS	2.00	12.5	-0.065	313.5	-18.8	-61.5
La_2S_3	3.00	-54.3	0.188	430.0	72.6	195.6
CeS	2.00	12.5	-0.065	311.3	-18.7	-62.9
WS_2	4.00	-628.1	1.627	432.3	632.8	2061.9
Na_2S_2	1.00	-	-	486.8	-	-
N						
Be_3N_2	2.00	91.9	-0.476	2921.1	-792.0	-779.1
BN	3.00	99.8	-0.345	3239.7	-607.4	-550.3
(CN)	3.00	-	-	3090.4	-	-

Na_3N	1.00	-	-	969.0	-	-
Mg_3N_2	2.00	47.9	-0.248	1593.3	-280.0	-346.4
AlN	3.00	158.4	-0.547	1961.6	-711.8	-852.9
Si_3N_4	4.00	42.7	-0.111	2292.6	-159.3	-177.9
K_3N	1.00	-	-	612.4	-	-
Ca_3N_2	2.00	36.9	-0.191	1084.7	-162.1	-230.5
ScN	3.00	155.2	-0.536	1363.6	-540.2	-
TiN	3.00	115.2	-0.398	1299.5	-387.0	-629.1
VN	3.00	62.5	-0.216	1238.0	-202.3	-350.0
CrN	3.00	-35.6	0.123	1218.2	113.9	197.1
Cr_2N	1.50	-13.2	0.091	681.4	52.8	130.2
Mn_4N	0.75	-5.9	0.082	344.0	25.8	-
Mn_5N_2	1.20	-20.4	0.177	531.2	82.4	-
Fe_2N	1.50	-	-	639.7	-	-
Fe_4N	0.75	-31.2	0.431	338.7	134.3	-
Co_3N	1.00	-31.4	0.326	421.4	123.7	380.4
NiN	3.00	-	-	1106.0	-	-
Cu_3N	1.00	-	-	392.9	-	-
Zn_3N_2	2.00	-98.8	0.512	717.3	309.9	722.3
GaN	3.00	-50.9	0.176	960.3	135.1	268.0
Ge_3N_4	4.00	-	-	1174.0	-	-
As_3N_5	5.00	-	-	1363.7	-	-
SeN_2	6.00	-	-	1503.3	-	-
YN	3.00	140.0	-0.484	781.3	-314.2	-677.7
ZrN	3.00	208.1	-0.719	764.1	-458.6	-1073.7
NbN	3.00	77.3	-0.267	752.1	-168.1	-416.0
MoN	3.00	-	-	731.3	-	-
RuN	3.00	-	-	698.7	-	-
Ag_3N	1.00	-	-	238.2	-	-
LaN	3.00	142.4	-0.492	525.8	-227.7	-641.1
CeN	3.00	166.4	-0.575	521.7	-264.1	-789.5
WN_2	6.00	-	-	759.1	-	-
NaN_3	1.00	-	-	179.8	-	-
KN_3	1.00	-	-	162.3	-	-
AgN_3	1.00	-	-	114.6	-	-
P		-				
Be_3P_2	2.00	-	-	1807.2	-	-

BP	3.00	-	-	1924.2	-	-
Na_3P	1.00	-	-	804.5	-	-
Mg_3P_2	2.00	-	-	1192.4	-	-
AlP	3.00	-	-	1387.3	-	-
Si_3P_4	4.00	-	-	1545.1	-	-
K_3P	1.00	-	-	542.3	-	-
Ca_3P_2	2.00	-	-	882.7	-	-
ScP	3.00	-	-	1058.9	-	-
TiP	3.00	-	-	1019.8	-	-
(VP)	3.00	-	-	981.6	-	-
CrP	3.00	-	-	969.1	-	-
MnP	3.00	-	-	935.9	-	-
Mn_2P	1.50	-	-	570.9	-	-
FeP	3.00	-	-	926.1	-	-
Fe_2P	1.50	-	-	563.6	-	-
Fe_3P	1.00	-	-	405.0	-	-
Co_2P	1.50	-	-	540.2	-	-
Ni_2P	1.50	-	-	542.0	-	-
Ni_3P	1.00	-	-	388.3	-	-
Ni_5P_2	1.20	-	-	452.5	-	-
CuP_2	6.00	-	-	1281.4	-	-
Cu_3P	1.00	-	-	362.8	-	-
Zn_3P_2	2.00	-	-	623.0	-	-
GaP	3.00	-	-	798.5	-	-
GeP	3.00	-	-	776.0	-	-
Ge_3P_4	4.00	-	-	940.9	-	-
As_3P_5	5.00	-	-	1059.0	-	-
$Se(P)_2$	6.00	-	-	1141.2	-	-
YP	3.00	-	-	670.7	-	-
ZrP_2	6.00	-	-	1049.9	-	-
NbP	3.00	-	-	649.0	-	-
MoP	3.00	-	-	633.5	-	-
RuP	3.00	-	-	608.9	-	-
AgP_2	6.00	-	-	947.0	-	-
AgP_3	9.00	-	-	1201.3	-	-
LaP	3.00	-	-	473.3	-	-
Ce_3P_4	4.00	-	-	590.9	-	-

WP_2	6.00	-	-	654.3	-	-
Cl						
$BeCl_2$	2.00	-323.2	1.675	670.7	957.1	1319.1
PCl_5	5.00	-1617.1	3.352	643.5	1849.0	2736.5
NaCl	1.00	-0.3	0.003	458.6	1.3	2.1
$MgCl_2$	2.00	-177.0	0.917	563.0	450.7	734.4
$AlCl_3$	3.00	-524.4	1.812	603.0	944.9	1570.3
KCl	1.00	24.1	-0.250	359.5	-82.1	-132.6
$CaCl_2$	2.00	-20.0	0.104	483.0	44.5	71.6
$ScCl_3$	3.00	-327.3	1.131	531.4	528.2	891.0
$TiCl_2$	2.00	-304.4	1.577	451.3	637.4	1322.4
$TiCl_3$	3.00	-499.7	1.726	521.3	793.0	1424.9
VCl_2	2.00	-362.8	1.880	439.9	742.5	1581.6
VCl_3	3.00	-641.9	2.218	511.2	1001.0	1950.2
$CrCl_2$	2.00	-412.8	2.139	436.1	838.3	1669.8
$CrCl_3$	3.00	-667.1	2.305	507.7	1034.2	1922.9
$MnCl_2$	2.00	-328.3	1.701	425.9	652.7	1335.8
$FeCl_2$	2.00	-466.5	2.417	422.9	921.4	1964.0
$FeCl_3$	3.00	-819.2	2.830	495.7	1243.3	2397.2
$CoCl_2$	2.00	-499.0	2.586	412.8	964.4	2144.4
$NiCl_2$	2.00	-509.8	2.642	413.6	987.0	2250.7
CuCl	1.00	-264.5	2.741	270.7	693.5	1990.5
$CuCl_2$	2.00	-593.1	3.074	398.7	1110.7	2513.7
$ZnCl_2$	2.00	-399.4	2.070	393.3	738.8	1522.3
$GaCl_3$	3.00	-698.4	2.413	456.6	985.2	1759.1
$AsCl_5$	5.00	-	-	531.4	-	-
$SeCl_4$	4.00	-	-	485.6	-	-
YCl_3	3.00	-225.5	0.779	411.8	289.8	550.3
$ZrCl_2$	2.00	-382.8	1.984	330.6	604.1	1375.5
$ZrCl_3$	3.00	-507.2	1.752	406.9	645.1	1357.6
$ZrCl_4$	4.00	-647.7	1.678	460.0	689.9	1330.6
$NbCl_5$	5.00	-1238.8	2.568	496.0	1128.7	2121.9
$NbCl_4$	4.00	-932.1	2.415	456.7	986.4	2065.6
$MoCl_4$	4.00	-1135.6	2.942	450.9	1188.0	-
$MoCl_5$	5.00	-1499.0	3.107	490.5	1352.3	2631.5

$MoCl_6$	6.00	-1915.4	3.309	521.0	1518.8	-
$RuCl_3$	3.00	-993.5	3.432	387.6	1209.0	2605.8
AgCl	1.00	-274.6	2.846	187.0	507.6	1967.2
$SnCl_2$	2.00	-482.6	2.501	282.7	658.7	1811.5
$LaCl_3$	3.00	-	-	327.8	-	-
$CeCl_3$	3.00	-168.4	0.582	326.2	175.0	462.8
WCl_2	2.00	-548.8	2.844	210.4	567.5	2093.4
WCl_4	4.00	-1177.6	3.051	329.2	925.6	2670.7
WCl_5	5.00	-1520.0	3.151	371.1	1066.7	2671.3
WCl_6	6.00	-1850.4	3.196	405.5	1173.0	2696.1
BO_2^-						
$NaBO_2$	1.00	-56.7	0.588	407.3	216.6	396.8
$Mg(BO_2)_2$	2.00	-	-	487.6	-	-
$Al(BO_2)_3$	3.00	-	-	517.4	-	-
KBO_2	1.00	-39.5	0.409	327.2	123.4	-
$Sc(BO_2)_3$	3.00	-	-	463.7	-	-
$Ti(BO_2)_4$	4.00	-	-	489.3	-	-
$V(BO_2)_5$	5.00	-	-	505.7	-	-
$Cr(BO_2)_6$	6.00	-	-	520.6	-	-
$Mn(BO_2)_3$	3.00	-	-	438.5	-	-
$Fe(BO_2)_2$	2.00	-	-	378.9	-	-
$Co(BO_2)_3$	3.00	-	-	429.1	-	-
$Ni(BO_2)_2$	2.00	-	-	371.4	-	-
$Cu(BO_2)_2$	2.00	-	-	359.3	-	-
$Zn(BO_2)_2$	2.00	-	-	355.0	-	-
$Ga(BO_2)_3$	3.00	-	-	405.8	-	-
$Ge(BO_2)_4$	4.00	-	-	439.6	-	-
$Y(BO_2)_3$	3.00	-	-	369.9	-	-
$Zr(BO_2)_4$	4.00	-	-	408.5	-	-
$Nb\ BO_2$	1.00	-	-	197.5	-	-
$MoBO_2$	1.00	-	-	193.2	-	-
$Ru(BO_2)_2$	2.00	-	-	287.1	-	-
$Ag\ BO_2$	1.00	-	-	177.9	-	-
$La(BO_2)_3$	3.00	-	-	300.8	-	-
$Ce(BO_2)_4$	4.00	-	-	344.3	-	-

$W(BO_2)_6$	6.00	-	-	364.9	-	-
$Be_3(BO_3)_2$	2.00	-	-	1111.7	-	-
$Ca_3(BO_3)_2$	2.00	-	-	676.1	-	-
CO_3^{2-}						
$BeCO_3$	2.00	-	-	776.6	-	-
$B_2(CO_3)_3$	3.00	-	-	797.5	-	-
Na_2CO_3	1.00	-43.9	0.455	505.7	203.3	359.8
$MgCO_3$	2.00	-120.0	0.622	635.8	339.5	617.3
$Al_2(CO_3)_3$	3.00	-	-	687.2	-	-
K_2CO_3	1.00	-34.3	0.356	387.8	125.3	220.7
$CaCO_3$	2.00	-3.3	0.017	535.6	8.1	14.8
$Sc_2(CO_3)_3$	3.00	-	-	595.7	-	-
$Ti(CO_3)_2$	4.00	-	-	638.6	-	-
$V_2(CO_3)_5$	5.00	-	-	666.8	-	-
$Cr(CO_3)_3$	6.00	-	-	693.1	-	-
$MnCO_3$	2.00	-315.4	1.635	466.3	680.1	1535.4
$Fe_2(CO_3)_3$	3.00	-	-	551.2	-	-
$FeCO_3$	2.00	-465.4	2.412	450.7	973.3	2302.3
$CoCO_3$	2.00	-495.3	2.567	450.7	1035.9	2533.2
$NiCO_3$	2.00	-514.2	2.665	451.6	1077.4	2693.1
$CuCO_3$	2.00	-	-	433.8	-	-
$ZnCO_3$	2.00	-400.6	2.076	427.5	798.8	2049.9
$Ga_2(CO_3)_3$	3.00	-	-	503.4	-	-
$Ge(CO_3)_2$	4.00	-	-	556.5	-	-
$Y_2(CO_3)_3$	3.00	-	-	449.4	-	-
$ZrCO_3$	2.00	-	-	354.4	-	-
Nb_2CO_3	1.00	-	-	218.1	-	-
Mo_2CO_3	1.00	-	-	212.8	-	-
Ru_2CO_3	1.00	-	-	204.5	-	-
Ag_2CO_3	1.00	-347.7	3.603	194.4	666.9	2706.2
$La_2(CO_3)_3$	3.00	-	-	351.2	-	-
$Ce_2(CO_3)_3$	3.00	-	-	349.4	-	-
$W(CO_3)_3$	6.00	-	-	441.9	-	-
PO_4^{3-}						

$Be_{3(}PO_{4)2}$	2.00	-	-	741.1	-	-
Na_3PO_4	1.00	-102.3	1.060	490.4	461.4	823.5
$Mg_3(PO_4)_2$	2.00	-217.6	1.128	611.8	595.5	918.3
Al PO_4	3.00	-477.8	1.651	659.3	929.6	1532.0
K_3 PO_4	1.00	-	-	378.8	-	-
$Ca_3(PO_4)_2$	2.00	-102.3	0.530	518.4	242.2	482.1
Sc PO_4	3.00	-	-	574.6	-	-
Ti $_3(PO_4)_4$	4.00	-	-	614.4	-	-
V_3 $(PO_4)_5$	5.00	-	-	640.5	-	-
$CrPO_4$	3.00	-	-	547.1	-	-
Mn PO_4	3.00	-	-	536.4	-	-
Mn3(PO_4)2	2.00	-	-	453.3	-	-
Fe PO_4	3.00	-908.2	3.138	533.1	1469.8	2755.8
$Co3(PO_{4)2}$	2.00	-	-	438.5	-	-
$Ni_3(PO_4)_2$	2.00	-		439.3	-	-
$Cu_3(PO_4)_2$	2.00	-	-	422.5	-	-
$Zn_3(PO_4)_2$	2.00	-509.3	2.639	416.5	992.1	2431.8
Ga PO_4	3.00	-	-	488.2	-	-
$Ge_3(PO_4)_4$	4.00	-	-	538.0	-	-
Y PO_4	3.00	-	-	437.3	-	-
Zr $_3(PO_4)_2$	2.00	-	-	346.9	-	-
Nb_3 PO_4	1.00	-	-	215.2	-	-
Mo_3PO_4	1.00	-	-	210.0	-	-
Ru_3 PO_4	1.00	-	-	201.9	-	-
Ag_3 PO_4	1.00	-	-	192.1	-	-
La PO_4	3.00	-	-	343.8	-	-
$CePO_4$	3.00	-	-	342.0	-	-
W $(PO_4)_2$	6.00	-	-	430.2	-	-
SO_4^{2-}						
Be SO_4	2.00	-232.3	1.204	510.1	542.4	948.6
Na_2 SO_4	1.00	-25.8	0.267	377.4	91.7	182.0
Mg SO_4	2.00	-151.1	0.783	445.3	312.6	589.1
Al_2($SO_4)_3$	3.00	-229.1	0.791	470.0	331.6	-
$AlK(SO_4)_2$	4.00	-403.3	1.045	415.2	391.7	-

K_2 SO_4	1.00	-0.1	0.002	307.6	0.4	0.9
$CaSO_4$	2.00	-12.6	0.065	393.7	23.3	48.6
Sc $_2(SO_4)_3$	3.00	-	-	425.3	-	-
Ti $(SO_4)_2$	4.00	-	-	446.7	-	-
$V_2(SO_4)_5$	5.00	-	-	460.3	-	-
Cr $2(SO_4)_3$	3.00	-674.0	2.328	410.0	863.1	1831.0
$MnSO_4$	2.00	-364.3	1.888	355.0	613.7	1396.5
$FeSO_4$	2.00	-500.9	2.596	352.9	839.2	2057.8
$Fe_2(SO_4)_3$	3.00	-851.2	2.941	402.1	1071.0	2284.7
Co SO_4	2.00	-539.3	2.795	345.8	887.1	2210.4
Ni SO_4	2.00	-562.0	2.912	346.4	925.7	2417.0
$CuSO_4$	2.00	-659.5	3.418	335.8	1055.9	2604.7
Zn SO_4	2.00	-450.2	2.333	332.0	713.2	1826.1
$Y_2(SO_4)_3$	3.00	-	-	345.1	-	-
$Zr(SO_{4)2}$	4.00	-	-	378.3	-	-
Nb_2SO_4	1.00	-	-	190.2	-	-
Mo_2SO_4	1.00	-	-	186.2	-	-
Ru_2SO_4	1.00	-	-	179.8	-	-
Ag_2 SO_4	1.00	-351.7	3.645	171.9	599.9	2347.9
La $_2(SO_4)_3$	3.00	-	-	284.1	-	-
$Ce_2(SO_4)_3$	3.00	-181.1	0.626	282.9	164.9	-
W $(SO_4)_3$	6.00	-	-	340.7	-	-

Na						
M_aX_b	n	Δ_rG (kJ mol^{-1})	EMF (V)	Capacity (m A h g^{-1})	Cal. Energy density (W h kg^{-1})	Cal. Energy density (W h L^{-1})
F						
BeF_2	2.00	-113.2	0.587	1140.3	338.2	450.6
LiF	1.00	41.4	-0.429	1033.2	-235.0	-343.0
MgF_2	2.00	-21.5	0.111	860.4	55.2	88.9
AlF_3	3.00	-207.8	0.718	957.5	377.4	587.9
KF	1.00	-8.5	0.088	461.3	29.1	50.1
CaF_2	2.00	83.0	-0.430	686.6	-185.9	-320.4

ScF_3	3.00	-99.1	0.342	788.7	161.0	245.6
TiF_3	3.00	-276.9	0.957	766.8	442.5	723.6
TiF_4	4.00	-626.2	1.623	865.5	806.0	1250.8
VF_3	3.00	-412.2	1.424	744.9	647.3	1109.6
CrF_3	3.00	-535.5	1.850	737.7	835.8	1490.6
MnF_2	2.00	-285.5	1.479	576.8	570.9	1120.9
MnF_3	3.00	-639.1	2.208	718.3	981.3	1728.2
FeF_2	2.00	-424.0	2.197	571.2	842.3	1674.3
FeF_3	3.00	-666.9	2.304	712.5	1018.9	1847.7
CoF_2	2.00	-445.4	2.308	553.0	865.7	1789.6
CoF_3	3.00	-919.9	3.178	693.6	1382.0	2530.5
NiF_2	2.00	-488.5	2.531	554.4	951.1	1996.3
CuF	1.00	-286.3	2.967	324.7	753.6	2251.2
CuF_2	2.00	-600.6	3.112	527.9	1130.9	2336.4
ZnF_2	2.00	-379.3	1.966	518.5	705.4	1538.1
GaF_3	3.00	-553.6	1.913	634.5	785.8	1546.3
RbF	1.00	-17.8	0.184	256.6	38.7	93.0
YF_3	3.00	5.8	-0.020	551.1	-7.5	-15.0
ZrF_2	2.00	-179.6	0.931	414.8	284.8	-
ZrF_3	3.00	-313.3	1.083	542.5	0.0	0.0
ZrF_4	4.00	-375.3	0.972	641.1	402.2	786.5
NbF_5	5.00	-1032.5	2.140	713.2	947.0	1524.8
RuF_3	3.00	-	-	508.7	-	-
RuF_5	5.00	-1950.2	4.043	683.5	1741.8	3209.8
AgF	1.00	-359.3	3.724	211.3	666.0	2199.3
SnF_2	2.00	-491.1	2.545	342.1	673.1	1670.0
LaF_3	3.00	-15.1	0.052	410.4	15.9	40.3
CeF_3	3.00	-82.9	0.286	407.9	86.5	223.3
O						
BeO-α	2.00	204.6	-1.060	2143.1	-800.6	-1020.1
B_2O_3	3.00	33.9	-0.117	2309.7	-90.7	-111.1
Li_2O	1.00	92.9	-0.962	1793.9	-680.0	-828.7
MgO microcrystal	2.00	193.8	-1.004	1329.9	-623.9	-923.5
Al_2O_3	3.00	227.9	-0.787	1577.2	-527.7	-754.4
SiO_2 quartz	4.00	105.3	-0.273	1784.3	-192.4	-247.9

SiO_2 high cristobalite	4.00	102.6	-0.266	1784.3	-187.4	-236.4
P_4O_{10}	5.00	-257.9	0.535	1888.2	385.4	471.9
K_2O	1.00	-26.7	0.277	569.1	105.8	169.6
CaO	2.00	227.8	-1.180	955.9	-620.0	-985.8
Sc_2O_3	3.00	346.5	-1.197	1166.0	-697.7	-1081.9
TiO	2.00	119.5	-0.619	839.3	-302.2	-550.5
Ti_2O_3	3.00	153.9	-0.532	1118.8	-303.4	-490.5
Ti_3O_5	3.33	146.6	-0.456	1198.6	-269.5	-421.7
TiO_2-R	4.00	138.1	-0.358	1342.3	-223.2	-336.5
TiO_2	4.00	137.8	-0.357	1342.3	-222.8	-335.9
TiO_2-A	4.00	131.9	-0.342	1342.3	-213.3	-317.9
VO	2.00	28.7	-0.149	800.7	-70.6	-142.3
V_2O_3	3.00	6.4	-0.022	1072.9	-12.4	-20.6
VO_2	4.00	567.5	-1.470	1292.6	-901.2	-1383.7
V_3O_5	3.33	-24.8	0.077	1151.2	44.7	-
V_2O_5	5.00	-229.0	0.475	1473.6	309.0	436.7
CrO_2	4.00	-206.1	0.534	1276.3	325.4	511.3
Cr_2O_3	3.00	-34.2	0.118	1058.0	65.5	110.9
Cr_3O_4 (Δ H=-1513 kJ mol^{-1})	2.67	9.7	-0.038	974.7	-19.9	-35.7
CrO_3	6.00	-613.9	1.061	1608.2	716.7	951.5
MnO_2	4.00	-285.9	0.741	1233.1	443.9	709.6
Mn_2O_3	3.00	-122.7	0.424	1018.6	230.4	392.3
MnO	2.00	-12.6	0.065	755.6	29.9	57.7
Mn_3O_4	2.67	-72.9	0.283	937.1	147.3	256.6
FeO	2.00	-124.1	0.643	746.1	292.6	580.6
Fe_2O_3 hematite	3.00	-192.2	0.664	1007.0	358.7	618.4
Fe_3O_4 magnetite	2.67	-162.2	0.630	926.1	325.3	576.7
CoO	2.00	-161.3	0.836	715.3	370.6	758.9
Co_3O_4	2.67	-242.7	0.943	890.4	476.1	883.0
NiO	2.00	-163.8	0.849	717.6	377.1	792.3
Ni_2O_3	3.00	-	-	972.3	-	-
CuO	2.00	-245.8	1.274	673.9	543.9	1137.8
Cu_2O	1.00	-114.8	1.189	374.6	337.2	894.7

ZnO	2.00	-55.0	0.285	658.6	119.9	246.7
Ga_2O_3	3.00	-64.1	0.221	857.9	109.4	205.3
GeO	2.00	-138.3	0.717	604.7	285.4	-
GeO_2	4.00	-229.6	0.595	1024.5	324.4	534.0
As_4O_6 octahedral	3.00	-275.1	0.950	812.8	455.2	786.8
As_2O_5	5.00	-547.6	1.135	1166.1	661.7	1048.3
SeO_2	4.00	-579.5	1.502	966.2	793.3	1309.9
Y_2O_3	3.00	345.1	-1.192	712.1	-527.0	-1024.6
ZrO_2	4.00	291.8	-0.756	870.0	-376.7	-695.8
NbO	2.00	16.4	-0.085	492.2	-29.5	-73.3
NbO_2	4.00	-10.5	0.027	858.3	13.4	25.1
Nb_2O_5	5.00	-55.9	0.116	1008.3	62.6	104.7
MoO_2	4.00	-218.0	0.565	837.9	275.4	528.5
MoO_3	6.00	-458.5	0.792	1117.2	451.8	736.9
RuO_2	4.00	-471.0	1.220	805.6	581.4	1150.9
RuO_4	8.00	-1349.8	1.749	1298.9	1074.4	1563.7
AgO	2.00	-389.3	2.018	432.7	636.7	1692.0
Ag_2O	1.00	-182.1	1.888	231.3	364.4	1271.5
Ag_2O_3	3.00	-624.0	2.156	609.7	863.0	-
La_2O_3	3.00	289.7	-1.001	493.6	-347.0	-837.0
CeO_2	4.00	273.6	-0.709	622.9	-287.8	-640.5
Ce_2O_3	3.00	289.9	-1.001	489.9	-345.4	-825.2
WO_2	4.00	-217.1	0.563	496.7	195.9	525.4
WO_3	6.00	-362.5	0.626	693.6	272.3	577.4
Li_2O_2	1.00	61.6	-0.639	1168.3	-372.7	-537.0
K_2O_2	1.00	-11.3	0.117	486.4	40.2	63.5
Ag_2O_2	1.00	-237.7	2.463	216.4	449.5	1636.0
LiO_2	1.00	-	-	688.3	-	-
KO_2	1.00	21.0	-0.218	377.0	-62.0	-103.0
CaO_2	1.00	385.7	-3.998	371.8	-1127.1	-2206.8
S						
BeS	2.00	-116.8	0.605	1304.9	372.7	500.6
B_2S_3	3.00	-400.9	1.385	1364.8	870.8	1053.0
Li_2S	1.00	44.6	-0.462	1166.6	-269.5	-343.4
MgS	2.00	-8.0	0.041	950.9	21.7	32.5

Al_2S_3	3.00	-204.7	0.707	1070.9	394.7	525.2
SiS_2	4.00	-487.0	1.262	1162.5	734.5	966.2
P_4S_3	1.50	-222.6	1.538	730.6	690.8	986.9
P_4S_7	3.50	-537.4	1.591	1077.1	890.9	1216.3
P_2S_5	5.00	-804.9	1.668	1205.8	988.9	1290.5
K_2S	1.00	7.1	-0.074	486.1	-25.2	-35.6
CaS	2.00	127.6	-0.661	743.0	-300.1	-471.0
Sc_2S_3	3.00	-	-	864.1	-	-
TiS_2	4.00	-297.4	0.771	957.2	405.1	645.3
TiS	2.00	-79.7	0.413	670.6	175.9	324.9
Ti_2S_3	3.00	-	-	837.8	-	-
VS	2.00	-	-	645.8	-	-
V_2S_3	3.00	-	-	811.8	-	-
VS_2	4.00	-	-	931.6	-	-
V_2S_5	5.00	-	-	1022.1	-	-
CrS	2.00	-175.4	0.909	637.7	374.6	-
Cr_2S_3	3.00	-440.8	1.523	803.3	724.2	1253.8
MnS	2.00	-131.4	0.681	616.1	274.5	506.8
MnS_2	4.00	-474.6	1.230	900.4	624.7	-
FeS	2.00	-249.4	1.292	609.7	517.4	1048.0
$FeS_{2(marcasite)}$	4.00	-543.5	1.408	893.6	712.3	1271.8
$FeS_{2(pyrite)}$	4.00	-532.7	1.380	893.6	698.2	1246.6
CoS	2.00	-	-	589.0	-	-
Co_2S_3	3.00	-	-	751.2	-	-
CoS_2	4.00	-554.0	1.435	871.1	715.6	1246.7
Co_3S_4	2.67	-304.1	1.182	702.8	518.3	-
NiS	2.00	-270.3	1.401	590.6	549.1	1175.0
Ni_3S_4	2.67	-369.1	1.435	704.5	629.9	1213.7
Ni_3S_2	1.33	-163.2	1.269	446.3	409.4	-
NiS_2	4.00	-574.9	1.490	872.8	743.5	-
CuS	2.00	-296.2	1.535	560.6	581.1	1219.1
Cu_2S	1.00	-131.8	1.366	336.8	356.9	965.7
ZnS	2.00	-148.5	0.770	550.0	287.6	577.9
Ga_2S_3	3.00	-271.8	0.939	682.4	404.3	733.5
GaS	2.00	-145.1	0.752	526.6	272.8	546.4
GeS	2.00	-278.3	1.442	511.9	513.0	1059.9

GeS_2	4.00	-545.0	1.412	783.8	661.9	1079.5
As_2S_3	3.00	-440.4	1.521	653.6	637.2	1147.0
Se_2S_6	6.00	-	-	918.1	-	-
Se_4S_4	2.00	-	-	482.8	-	-
RuS_2	4.00	-	-	648.9	-	-
Y_2S_3	3.00	-	-	586.9	-	-
ZrS_2	4.00	-129.6	0.336	690.1	145.5	266.7
NbS_2	4.00	-	-	682.7	-	-
MoS_2	4.00	-473.7	1.227	669.7	522.1	1040.7
Mo_2S_3	3.00	-385.4	1.331	558.2	502.6	1121.3
$Ag_2S_{(argentite)}$	1.00	-154.6	1.602	216.3	292.3	1051.3
LaS	2.00	101.7	-0.527	313.5	-130.2	-362.7
La_2S_3	3.00	79.5	-0.275	430.0	-86.2	-202.0
CeS	2.00	101.7	-0.527	311.3	-129.5	-368.9
WS_2	4.00	-449.7	1.165	432.3	367.5	980.3
Li_2S_2	1.00	-	-	376.6	-	-
N						
Be_3N_2	2.00	240.1	-1.244	2921.1	-1036.9	-1231.3
BN	3.00	322.2	-1.113	3239.7	-954.2	-1084.9
(CN)	3.00	-	-	3090.4	-	-
Li_3N	1.00	74.1	-0.768	2308.5	-595.1	-
Mg_3N_2	2.00	196.1	-1.016	1593.3	-684.3	-910.9
AlN	3.00	380.8	-1.315	1961.6	-961.9	-1263.7
Si_3N_4	4.00	339.2	-0.879	2292.6	-679.3	-860.1
K_3N	1.00	-	-	612.4	-	-
Ca_3N_2	2.00	185.2	-0.960	1084.7	-539.2	-780.4
ScN	3.00	377.5	-1.304	1363.6	-819.7	-
TiN	3.00	337.6	-1.166	1299.5	-716.6	-1130.0
VN	3.00	284.8	-0.984	1238.0	-590.8	-968.5
CrN	3.00	186.8	-0.645	1218.2	-384.4	-630.4
Cr_2N	1.50	98.0	-0.677	681.4	-291.1	-615.4
Mn_4N	0.75	49.7	-0.687	344.0	-182.4	-
Mn_5N_2	1.20	68.5	-0.592	531.2	-215.9	-
Fe_2N	1.50	-	-	639.7	-	-
Fe_4N	0.75	24.4	-0.337	338.7	-88.4	-
Co_3N	1.00	42.7	-0.443	421.4	-137.0	-352.7

NiN	3.00	-	-	1106.0	-	-
Cu_3N	1.00	-	-	392.9	-	-
Zn_3N_2	2.00	49.4	-0.256	717.3	-113.7	-230.9
GaN	3.00	171.5	-0.592	960.3	-312.0	-561.6
Ge_3N_4	4.00	-	-	1174.0	-	-
As_3N_5	5.00	-	-	1363.7	-	-
SeN_2	6.00	-	-	1503.3	-	-
YN	3.00	362.3	-1.252	781.3	-585.6	-1124.8
ZrN	3.00	430.5	-1.487	764.1	-686.4	-1391.3
NbN	3.00	299.7	-1.035	752.1	-473.3	-994.2
MoN	3.00	-	-	731.3	-	-
RuN	3.00	-	-	698.7	-	-
Ag_3N	1.00	-	-	238.2	-	-
LaN	3.00	364.8	-1.260	525.8	-456.7	-1080.0
CeN	3.00	388.7	-1.343	521.7	-484.0	-1191.3
WN_2	6.00	-	-	759.1	-	-
LiN_3	1.00	-	-	201.5	-	-
KN_3	1.00	-	-	162.3	-	-
AgN_3	1.00	-	-	114.6	-	-
P						
Be_3P_2	2.00	-	-	1807.2	-	-
BP	3.00	-	-	1924.2	-	-
Li_3P	1.00	-	-	1552.3	-	-
Mg_3P_2	2.00	-	-	1192.4	-	-
AlP	3.00	-	-	1387.3	-	-
Si_3P_4	4.00	-	-	1545.1	-	-
K_3P	1.00	-	-	542.3	-	-
Ca_3P_2	2.00	-	-	882.7	-	-
ScP	3.00	-	-	1058.9	-	-
TiP	3.00	-	-	1019.8	-	-
(VP)	3.00	-	-	981.6	-	-
CrP	3.00	-	-	969.1	-	-
MnP	3.00	-	-	935.9	-	-
Mn_2P	1.50	-	-	570.9	-	-
FeP	3.00	-	-	926.1	-	-
Fe_2P	1.50	-	-	563.6	-	-
Fe_3P	1.00	-	-	405.0	-	-
Co_2P	1.50	-	-	540.2	-	-

Ni_2P	1.50	-	-	542.0	-	-
Ni_3P	1.00	-	-	388.3	-	-
Ni_5P_2	1.20	-	-	452.5	-	-
CuP_2	6.00	-	-	1281.4	-	-
Cu_3P	1.00	-	-	362.8	-	-
Zn_3P_2	2.00	-	-	623.0	-	-
GaP	3.00	-	-	798.5	-	-
GeP	3.00	-	-	776.0	-	-
Ge_3P_4	4.00	-	-	940.9	-	-
As_3P_5	5.00	-	-	1059.0	-	-
$Se(P)_2$	6.00	-	-	1141.2	-	-
YP	3.00	-	-	670.7	-	-
ZrP_2	6.00	-	-	1049.9	-	-
NbP	3.00	-	-	649.0	-	-
MoP	3.00	-	-	633.5	-	-
RuP	3.00	-	-	608.9	-	-
AgP_2	6.00	-	-	947.0	-	-
AgP_3	9.00	-	-	1201.3	-	-
LaP	3.00	-	-	473.3	-	-
Ce_3P_4	4.00	-	-	590.9	-	-
WP_2	6.00	-	-	654.3	-	-
Cl						
$BeCl_2$	2.00	-322.6	1.672	670.7	711.8	1001.6
PCl_5	5.00	-1615.6	3.349	643.5	1388.6	2061.8
LiCl	1.00	0.3	-0.003	632.2	-1.3	-1.9
$MgCl_2$	2.00	-176.4	0.914	563.0	347.0	554.6
$AlCl_3$	3.00	-523.5	1.809	603.0	718.8	1164.6
KCl	1.00	24.4	-0.253	359.5	-69.5	-110.7
$CaCl_2$	2.00	-19.4	0.101	483.0	34.3	54.4
$ScCl_3$	3.00	-326.4	1.128	531.4	411.6	675.9
$TiCl_2$	2.00	-303.8	1.574	451.3	512.2	988.8
$TiCl_3$	3.00	-498.8	1.723	521.3	620.8	1069.8
VCl_2	2.00	-362.2	1.877	439.9	599.5	1181.9
VCl_3	3.00	-641.0	2.215	511.2	786.9	1441.3
$CrCl_2$	2.00	-412.2	2.136	436.1	678.0	1271.2
$CrCl_3$	3.00	-666.2	2.302	507.7	814.1	1440.4

$MnCl_2$	2.00	-327.7	1.698	425.9	529.8	1015.1
$FeCl_2$	2.00	-465.9	2.414	422.9	749.2	1481.0
$FeCl_3$	3.00	-818.3	2.827	495.7	983.3	1789.3
$CoCl_2$	2.00	-498.4	2.583	412.8	787.4	1609.0
$NiCl_2$	2.00	-509.2	2.639	413.6	805.6	1677.4
CuCl	1.00	-264.2	2.738	270.7	601.6	1541.3
$CuCl_2$	2.00	-592.5	3.070	398.7	912.2	1892.9
$ZnCl_2$	2.00	-398.8	2.067	393.3	607.7	1174.9
$GaCl_3$	3.00	-697.5	2.410	456.6	790.7	1360.7
$AsCl_5$	5.00	-	-	531.4	-	-
$SeCl_4$	4.00	-	-	485.6	-	-
YCl_3	3.00	-224.6	0.776	411.8	236.1	427.5
$ZrCl_2$	2.00	-382.2	1.981	330.6	510.1	1075.6
$ZrCl_3$	3.00	-506.3	1.749	406.9	527.6	1035.0
$ZrCl_4$	4.00	-646.5	1.675	460.0	552.6	1008.7
$NbCl_5$	5.00	-1237.3	2.565	496.0	892.4	1593.5
$NbCl_4$	4.00	-930.9	2.412	456.7	791.5	1537.7
$MoCl_4$	4.00	-1134.4	2.939	450.9	955.7	-
$MoCl_5$	5.00	-1497.5	3.104	490.5	1071.7	1964.5
$MoCl_6$	6.00	-1913.6	3.306	521.0	1190.2	-
$RuCl_3$	3.00	-992.6	3.429	387.6	997.5	1997.7
AgCl	1.00	-274.3	2.843	187.0	458.1	1540.0
$SnCl_2$	2.00	-482.0	2.498	282.7	568.3	1403.3
$LaCl_3$	3.00	-	-	327.8	-	-
$CeCl_3$	3.00	-167.5	0.579	326.2	147.5	349.3
WCl_2	2.00	-548.2	2.841	210.4	506.4	1616.1
WCl_4	4.00	-1176.4	3.048	329.2	782.5	1977.0
WCl_5	5.00	-1518.5	3.148	371.1	886.0	1993.7
WCl_6	6.00	-1848.6	3.193	405.5	960.7	2014.8
BO_2^-						
$LiBO_2$	1.00	56.7	-0.588	538.7	-216.6	-
$Mg(BO_2)_2$	2.00	-	-	487.6	-	-
$Al(BO_2)_3$	3.00	-	-	517.4	-	-
KBO_2	1.00	-	-	327.2	-	-
$Sc(BO_2)_3$	3.00	-	-	463.7	-	-

$Ti(BO_2)_4$	4.00	-	-	489.3	-	-
$V(BO_2)_5$	5.00	-	-	505.7	-	-
$Cr(BO_2)_6$	6.00	-	-	520.6	-	-
$Mn(BO_2)_3$	3.00	-	-	438.5	-	-
$Fe(BO_2)_2$	2.00	-	-	378.9	-	-
$Co(BO_2)_3$	3.00	-	-	429.1	-	-
$Ni(BO_2)_2$	2.00	-	-	371.4	-	-
$Cu(BO_2)_2$	2.00	-	-	359.3	-	-
$Zn(BO_2)_2$	2.00	-	-	355.0	-	-
$Ga(BO_2)_3$	3.00	-	-	405.8	-	-
$Ge(BO_2)_4$	4.00	-	-	439.6	-	-
$Y(BO_2)_3$	3.00	-	-	369.9	-	-
$Zr(BO_2)_4$	4.00	-	-	408.5	-	-
$Nb\ BO_2$	1.00	-	-	197.5	-	-
$MoBO_2$	1.00	-	-	193.2	-	-
$Ru(BO_2)_2$	2.00	-	-	287.1	-	-
$Ag\ BO_2$	1.00	-	-	177.9	-	-
$La(BO_2)_3$	3.00	-	-	300.8	-	-
$Ce(BO_2)_4$	4.00	-	-	344.3	-	-
$W(BO_2)_6$	6.00	-	-	364.9	-	-
$Be_3(BO_3)_2$	2.00	-	-	1111.8	-	-
$Ca_3(BO_3)_2$	2.00	-	-	676.1	-	-
CO_3^{2-}						
$Be\ CO_3$	2.00	-	-	776.6	-	-
$B_2(CO_3)_3$	3.00	-	-	797.5	-	-
$Li_2\ CO_3$	1.00	43.9	-0.455	725.4	-203.3	-
$Mg\ CO_3$	2.00	-32.3	0.167	635.8	68.9	119.0
$Al_2(\ CO_3)_3$	3.00	-	-	687.2	-	-
$K_2\ CO_3$	1.00	9.5	-0.099	387.8	-28.8	-49.2
$CaCO_3$	2.00	84.4	-0.437	535.6	-160.5	-280.4
$Sc_2(CO_{3)3}$	3.00	-	-	595.7	-	-
$Ti(CO_3)_2$	4.00	-	-	638.6	-	-
$V_2(CO_3)_5$	5.00	-	-	666.8	-	-
$Cr(CO_3)_3$	6.00	-	-	693.1	-	-

$MnCO_3$	2.00	-227.7	1.180	466.3	393.0	806.1
$Fe_2(CO_3)_3$	3.00	-	-	551.2	-	-
$FeCO_3$	2.00	-377.7	1.957	450.7	636.2	1352.7
$Co\ CO_3$	2.00	-407.6	2.112	450.7	686.6	1495.3
$Ni\ CO_3$	2.00	-426.5	2.210	451.6	719.4	1591.5
$CuCO_3$	2.00	-	-	433.8	-	-
$Zn\ CO_3$	2.00	-312.8	1.621	427.5	507.0	1148.2
$Ga_2(CO_3)_3$	3.00	-	-	503.4	-	-
$Ge(CO_3)_2$	4.00	-	-	556.5	-	-
$Y_2(CO_3)_3$	3.00	-	-	449.4	-	-
$ZrCO_3$	2.00	-	-	354.4	-	-
$Nb_2\ CO_3$	1.00	-	-	218.1	-	-
Mo_2CO_3	1.00	-	-	212.8	-	-
Ru_2CO_3	1.00	-	-	204.5	-	-
$Ag_2\ CO_3$	1.00	-303.8	3.149	194.4	524.6	1819.2
$La\ _2(CO_3)_3$	3.00	-	-	351.2	-	-
$Ce_2(CO_3)_3$	3.00	-	-	349.4	-	-
$W\ (CO_3)_3$	6.00	-	-	441.9	-	-
PO_4^{3-}						
$Be_3(PO_4)_2$	2.00	-	-	741.1	-	-
Li_3PO_4(ΔH=-698.6 kJ mol^{-1})	1.00	-363.4	3.767	694.4	1639.1	2595.3
$Mg_3(PO_4)_2$	2.00	-13.0	0.067	611.8	27.0	41.3
$Al\ PO_4$	3.00	-170.9	0.590	659.3	248.6	399.7
$K_3\ PO_4$	1.00	-	-	378.8	-	-
$Ca_3(PO_4)_2$	2.00	102.4	-0.530	518.4	-190.3	-353.9
$Sc\ PO_4$	3.00	-	-	574.6	-	-
$Ti\ _3(PO_4)_4$	4.00	-	-	614.4	-	-
$V_3\ (PO_4)_5$	5.00	-	-	640.5	-	-
$CrPO_4$	3.00	-	-	547.1	-	-
$Mn\ PO_4$	3.00	-	-	536.4	-	-
$Mn_3(\ PO_4\ )_2$	2.00	-	-	453.3	-	-
$Fe\ PO_4$	3.00	-601.3	2.077	533.1	759.9	1350.7
$Co3(PO_{4)2}$	2.00	-	-	438.5	-	-

$Ni_3(PO_4)_2$	2.00	-	-	439.3	-	-
$Cu_3(PO_4)_2$	2.00	-	-	422.5	-	-
$Zn_3(PO_4)_2$	2.00	-304.7	1.579	416.5	484.5	1063.4
Ga PO_4	3.00	-	-	488.2	-	-
$Ge_3(PO_4)_4$	4.00	-	-	538.0	-	-
Y PO_4	3.00	-	-	437.3	-	-
Zr $_3(PO_4)_2$	2.00	-	-	346.9	-	-
Nb_3 PO_4	1.00	-	-	215.2	-	-
Mo_3PO_4	1.00	-	-	210.0	-	-
Ru_3 PO_4	1.00	-	-	201.9	-	-
Ag_3 PO_4	1.00	-	-	192.1	-	-
La PO_4	3.00	-	-	343.8	-	-
$CePO_4$	3.00	-	-	342.0	-	-
W $(PO_4)_2$	6.00	-	-	430.2	-	-
SO_4^{2-}						
Be SO_4	2.00	-180.8	0.937	510.1	332.5	561.6
Li_2 SO_4	1.00	25.8	-0.267	487.5	-91.7	-162.3
Mg SO_4	2.00	-99.6	0.516	445.3	166.3	298.6
$Al_2($ $SO_4)_3$	3.00	-151.8	0.524	470.0	175.7	-
$AlK(SO_4)_2$	4.00	-300.3	0.778	415.2	238.2	-
K_2 SO_4	1.00	25.6	-0.265	307.6	-64.6	-126.0
$CaSO_4$	2.00	38.9	-0.202	393.7	-59.3	-115.7
Sc $_2(SO_4)_3$	3.00	-	-	425.3	-	-
Ti $(SO_4)_2$	4.00	-	-	446.7	-	-
$V_2(SO_4)_5$	5.00	-	-	460.3	-	-
Cr $2(SO_4)_3$	3.00	-596.7	2.062	410.0	625.4	1233.7
$MnSO_4$	2.00	-312.8	1.621	355.0	441.1	925.6
$FeSO_4$	2.00	-449.4	2.329	352.9	630.8	1402.3
$Fe_2(SO_4)_3$	3.00	-774.0	2.674	402.1	799.5	1585.5
Co SO_4	2.00	-487.8	2.528	345.8	674.2	1519.4
Ni SO_4	2.00	-510.5	2.645	346.4	706.4	1649.0
$CuSO_4$	2.00	-608.0	3.151	335.8	821.5	1841.0
Zn SO_4	2.00	-398.7	2.066	332.0	533.9	1232.1
$Y_2(SO_4)_3$	3.00	-	-	345.1	-	-

$Zr(SO_4)_2$	4.00	-	-	378.3	-	-
Nb_2SO_4	1.00	-	-	190.2	-	-
Mo_2SO_4	1.00	-	-	186.2	-	-
Ru_2SO_4	1.00	-	-	179.8	-	-
$Ag_2\ SO_4$	1.00	-325.9	3.378	171.9	506.1	1730.7
$La\ _2(SO_4)_3$	3.00	-	-	284.1	-	-
$Ce_2(SO_4)_3$	3.00	-103.8	0.359	282.9	81.7	-
$W\ (SO_4)_3$	6.00	-	-	340.7	-	-

Mg						
M_aX_b	n	Δ_rG (kJ mol^{-1})	EMF (V)	Capacity (m A h g^{-1})	Cal. Energy density (W h kg^{-1})	Cal. Energy density (W h L^{-1})
F						
BeF_2	2.00	-91.7	0.475	1140.3	357.2	700.4
NaF	1.00	10.8	-0.111	638.3	-55.2	-135.1
LiF	1.00	52.2	-0.540	1033.2	-380.3	-951.0
AlF_3	3.00	-175.6	0.606	957.5	404.9	1014.5
KF	1.00	2.3	-0.023	461.3	-8.9	-20.5
CaF_2	2.00	104.5	-0.542	686.6	-283.5	-753.3
ScF_3	3.00	-66.8	0.231	788.7	134.1	299.7
TiF_3	3.00	-244.7	0.845	766.8	480.9	1210.0
TiF_4	4.00	-583.2	1.511	865.5	939.3	2242.6
VF_3	3.00	-380.0	1.313	744.9	731.0	1988.8
CrF_3	3.00	-503.2	1.738	737.7	961.0	2814.8
MnF_2	2.00	-264.0	1.368	576.8	625.5	1964.2
MnF_3	3.00	-606.8	2.097	718.3	1136.0	3204.9
FeF_2	2.00	-402.5	2.086	571.2	946.3	3027.6
FeF_3	3.00	-634.7	2.193	712.5	1180.8	3516.4
CoF_2	2.00	-423.9	2.197	553.0	971.3	3296.7
CoF_3	3.00	-887.7	3.067	693.6	1618.1	4848.5
NiF_2	2.00	-467.0	2.420	554.4	1072.1	3753.9
CuF	1.00	-275.6	2.856	324.7	808.3	4111.1
CuF_2	2.00	-579.1	3.001	527.9	1278.2	4234.3

ZnF_2	2.00	-357.8	1.854	518.5	778.3	2832.9
GaF_3	3.00	-521.4	1.801	634.5	887.5	2936.0
RbF	1.00	-7.0	0.073	256.6	16.7	53.7
YF_3	3.00	38.1	-0.131	551.1	-58.0	-184.0
ZrF_2	2.00	-158.1	0.819	414.8	286.1	-
ZrF_3	3.00	-281.1	0.971	542.5	422.8	1400.1
ZrF_4	4.00	-332.3	0.861	641.1	427.7	1404.6
NbF_5	5.00	-978.8	2.029	713.2	1093.4	2600.4
RuF_3	3.00	-	-	508.7	-	-
RuF_5	5.00	-1896.5	3.931	683.5	2051.2	6180.7
AgF	1.00	-348.6	3.612	211.3	696.4	3376.9
SnF_2	2.00	-469.6	2.434	342.1	720.7	2702.3
LaF_3	3.00	17.1	-0.059	410.4	-20.5	-87.8
CeF_3	3.00	-50.6	0.175	407.9	60.2	265.5
O						
BeO-α	2.00	10.8	-0.056	2143.1	-60.8	-134.6
B_2O_3	3.00	-256.8	0.887	2309.7	1000.9	2060.0
Na_2O	1.00	-96.9	1.004	864.9	623.9	1303.8
Li_2O	1.00	-4.0	0.042	1793.9	41.5	78.0
Al_2O_3	3.00	-62.8	0.217	1577.2	199.6	516.4
SiO_2 quartz	4.00	-282.3	0.731	1784.3	721.4	1532.7
SiO_2 high cristobalite	4.00	-285.0	0.738	1784.3	728.3	1473.9
P_4O_{10}	5.00	-742.4	1.539	1888.2	1565.5	3020.3
K_2O	1.00	-123.6	1.281	569.1	579.5	1270.0
CaO	2.00	34.0	-0.176	955.9	-117.5	-306.9
Sc_2O_3	3.00	55.8	-0.193	1166.0	-146.9	-398.9
TiO	2.00	-74.3	0.385	839.3	234.1	767.6
Ti_2O_3	3.00	-136.9	0.473	1118.8	350.9	1027.5
Ti_3O_5	3.33	-176.4	0.548	1198.6	425.9	1198.2
TiO_2-R	4.00	-249.5	0.647	1342.3	539.5	1471.0
TiO_2	4.00	-249.8	0.647	1342.3	540.1	1472.6
TiO_2-A	4.00	-255.7	0.662	1342.3	552.8	1466.0
VO	2.00	-165.1	0.856	800.7	502.6	2028.1
V_2O_3	3.00	-284.3	0.982	1072.9	708.9	2171.7
VO_2	4.00	179.9	-0.466	1292.6	-379.8	-1061.1

V_3O_5	3.33	-347.8	1.082	1151.2	818.0	-
V_2O_5	5.00	-713.5	1.479	1473.6	1306.5	3191.2
CrO_2	4.00	-593.7	1.538	1276.3	1243.7	3653.0
Cr_2O_3	3.00	-324.9	1.122	1058.0	802.6	2539.7
Cr_3O_4 (ΔH=-1513 kJ mol^{-1})	2.67	-248.7	0.967	974.7	653.4	2253.0
CrO_3	6.00	-1195.3	2.065	1608.2	1920.3	4203.6
MnO_2	4.00	-673.5	1.745	1233.1	1380.2	4149.8
Mn_2O_3	3.00	-413.4	1.428	1018.6	995.1	3123.5
MnO	2.00	-206.4	1.070	755.6	602.0	2108.3
Mn_3O_4	2.67	-331.3	1.288	937.1	846.9	2675.2
FeO	2.00	-317.9	1.647	746.1	918.4	3401.8
Fe_2O_3 hematite	3.00	-482.9	1.668	1007.0	1153.3	3706.6
Fe_3O_4 magnetite	2.67	-420.6	1.635	926.1	1066.2	3479.9
CoO	2.00	-355.1	1.840	715.3	994.0	3850.1
Co_3O_4	2.67	-501.1	1.947	890.4	1235.3	4379.3
NiO	2.00	-357.6	1.853	717.6	1003.4	4137.1
Ni_2O_3	3.00	-	-	972.3	-	-
CuO	2.00	-439.6	2.278	673.9	1175.8	4592.2
Cu_2O	1.00	-211.7	2.194	374.6	702.4	3108.0
ZnO	2.00	-248.8	1.289	658.6	653.9	2423.4
Ga_2O_3	3.00	-354.8	1.226	857.9	757.1	2693.0
GeO	2.00	-332.1	1.721	604.7	816.8	-
GeO_2	4.00	-617.2	1.599	1024.5	1118.7	3260.0
As_4O_6 octahedral	3.00	-565.8	1.955	812.8	1161.0	3343.5
As_2O_5	5.00	-1032.1	2.139	1166.1	1631.9	4656.9
SeO_2	4.00	-967.1	2.506	966.2	1683.6	4792.1
Y_2O_3	3.00	54.4	-0.188	712.1	-101.1	-347.7
ZrO_2	4.00	-95.8	0.248	870.0	154.9	535.8
NbO	2.00	-177.4	0.919	492.2	369.8	1704.5
NbO_2	4.00	-398.1	1.032	858.3	637.3	2250.4
Nb_2O_5	5.00	-540.4	1.120	1008.3	775.0	2320.1
MoO_2	4.00	-605.6	1.569	837.9	952.8	3523.5
MoO_3	6.00	-1039.9	1.796	1117.2	1332.1	3980.0

RuO_2	4.00	-858.6	2.225	805.6	1312.8	5091.4
RuO_4	8.00	-2125.0	2.753	1298.9	2250.5	5562.9
AgO	2.00	-583.1	3.022	432.7	1093.2	5310.8
Ag_2O	1.00	-279.0	2.892	231.3	605.5	3357.7
Ag_2O_3	3.00	-914.7	3.160	609.7	1509.4	-
La_2O_3	3.00	-1.0	0.004	493.6	1.5	6.3
CeO_2	4.00	-114.0	0.295	622.9	143.5	611.1
Ce_2O_3	3.00	-0.8	0.003	489.9	1.2	5.0
WO_2	4.00	-604.7	1.567	496.7	635.2	3502.8
WO_3	6.00	-943.9	1.630	693.6	860.3	3535.8
Na_2O_2	1.00	-	-	687.4	-	-
K_2O_2	1.00	-	-	486.4	-	-
Ag_2O_2	1.00	-	-	216.4	-	-
S						
BeS	2.00	-108.8	0.564	1304.9	462.2	962.8
B_2S_3	3.00	-388.9	1.344	1364.8	1132.8	1941.9
Na_2S	1.00	4.0	-0.041	686.8	-21.7	-39.7
Li_2S	1.00	48.6	-0.504	1166.6	-384.3	-867.4
Al_2S_3	3.00	-192.7	0.666	1070.9	479.9	920.6
SiS_2	4.00	-471.0	1.220	1162.5	929.0	1788.0
P_4S_3	1.50	-216.6	1.497	730.6	821.4	1600.5
P_4S_7	3.50	-523.4	1.550	1077.1	1121.5	2263.1
P_2S_5	5.00	-784.9	1.627	1205.8	1268.3	2430.3
K_2S	1.00	11.1	-0.115	486.1	-45.8	-79.7
CaS	2.00	135.6	-0.703	743.0	-390.5	-900.3
Sc_2S_3	3.00	-	-	864.1	-	-
TiS_2	4.00	-281.4	0.729	957.2	486.7	1277.2
TiS	2.00	-71.7	0.372	670.6	191.1	573.4
Ti_2S_3	3.00	-	-	837.8	-	-
VS	2.00	-	-	645.8	-	-
V_2S_3	3.00	-	-	811.8	-	-
VS_2	4.00	-	-	931.6	-	-
V_2S_5	5.00	-	-	1022.1	-	-
CrS	2.00	-167.4	0.867	637.7	429.0	-
Cr_2S_3	3.00	-428.8	1.481	803.3	872.2	2506.0
MnS	2.00	-123.4	0.639	616.1	308.0	887.8

MnS_2	4.00	-458.6	1.188	900.4	759.7	-
FeS	2.00	-241.4	1.251	609.7	597.6	2051.3
$FeS_{2(marcasite)}$	4.00	-527.5	1.367	893.6	869.2	2825.0
$FeS_{2(pyrite)}$	4.00	-516.7	1.339	893.6	851.4	2767.1
CoS	2.00	-	-	589.0	-	-
Co_2S_3	3.00	-	-	751.2	-	-
CoS_2	4.00	-538.0	1.394	871.1	870.4	2640.6
Co_3S_4	2.67	-293.4	1.140	702.8	607.8	-
NiS	2.00	-262.3	1.359	590.6	633.2	2390.0
Ni_3S_4	2.67	-358.4	1.393	704.5	743.8	2494.4
Ni_3S_2	1.33	-157.9	1.227	446.3	455.5	-
NiS_2	4.00	-558.9	1.448	872.8	905.6	-
CuS	2.00	-288.2	1.493	560.6	667.6	2349.7
Cu_2S	1.00	-127.8	1.325	336.8	387.0	1674.3
ZnS	2.00	-140.5	0.728	550.0	320.5	1028.2
Ga_2S_3	3.00	-259.8	0.898	682.4	467.9	1366.5
GaS	2.00	-137.1	0.711	526.6	302.1	943.8
GeS	2.00	-270.3	1.401	511.9	582.0	1899.8
GeS_2	4.00	-529.0	1.371	783.8	792.7	2001.8
As_2S_3	3.00	-428.4	1.480	653.6	746.2	2105.0
Se_2S_6	6.00	-	-	918.1	-	-
Se_4S_4	2.00	-	-	482.8	-	-
RuS_2	4.00	-	-	648.9	-	-
Y_2S_3	3.00	-	-	586.9	-	-
ZrS_2	4.00	-113.6	0.294	690.1	154.7	463.2
NbS_2	4.00	-683.6	1.771	682.7	923.4	2982.9
MoS_2	4.00	-457.7	1.186	669.7	609.2	2133.1
Mo_2S_3	3.00	-373.4	1.290	558.2	574.6	2287.2
Ag_2S(argentite)	1.00	-150.6	1.561	216.3	307.4	1733.3
LaS	2.00	109.7	-0.568	313.5	-156.0	-685.4
La_2S_3	3.00	91.5	-0.316	430.0	-113.7	-429.6
CeS	2.00	109.7	-0.568	311.3	-155.1	-705.9
WS_2	4.00	-433.7	1.124	432.3	406.2	1988.1
Na_2S_2	1.00	-	-	486.8	-	-
N						

Be_3N_2	2.00	44.0	-0.228	2921.1	-286.5	-588.9
BN	3.00	28.0	-0.097	3239.7	-126.7	-239.9
(CN)	3.00	-	-	3090.4	-	-
Na_3N	1.00	-	-	969.0	-	-
Li_3N	1.00	-24.0	0.248	2308.5	280.0	590.0
AlN	3.00	86.6	-0.299	1961.6	-310.4	-716.2
Si_3N_4	4.00	-53.1	0.137	2292.6	154.6	345.1
K_3N	1.00	-	-	612.4	-	-
Ca_3N_2	2.00	-11.0	0.057	1084.7	41.3	93.7
ScN	3.00	83.3	-0.288	1363.6	-242.5	-
TiN	3.00	43.4	-0.150	1299.5	-122.5	-366.5
VN	3.00	-9.4	0.032	1238.0	25.7	82.4
CrN	3.00	-107.5	0.371	1218.2	291.3	928.0
Cr_2N	1.50	-49.1	0.339	681.4	176.7	712.1
Mn_4N	0.75	-23.9	0.330	344.0	98.1	-
Mn_5N_2	1.20	-49.2	0.425	531.2	181.8	-
Fe_2N	1.50	-	-	639.7	-	-
Fe_4N	0.75	-49.2	0.680	338.7	199.6	-
Co_3N	1.00	-55.4	0.574	421.4	203.0	908.4
NiN	3.00	-	-	1106.0	-	-
Cu_3N	1.00	-	-	392.9	-	-
Zn_3N_2	2.00	-146.7	0.760	717.3	411.6	1567.9
GaN	3.00	-122.7	0.424	960.3	283.6	982.2
Ge_3N_4	4.00	-	-	1174.0	-	-
As_3N_5	5.00	-	-	1363.7	-	-
SeN_2	6.00	-	-	1503.3	-	-
YN	3.00	68.1	-0.235	781.3	-135.8	-480.8
ZrN	3.00	136.3	-0.471	764.1	-267.1	-1056.6
NbN	3.00	5.5	-0.019	752.1	-10.6	-45.1
MoN	3.00	-	-	731.3	-	-
RuN	3.00	-	-	698.7	-	-
Ag_3N	1.00	-	-	238.2	-	-
LaN	3.00	70.6	-0.244	525.8	-103.5	-448.7
CeN	3.00	94.5	-0.326	521.7	-137.7	-648.0
WN_2	6.00	-	-	759.1	-	-
P						
Be_3P_2	2.00	-	-	1807.2	-	-
BP	3.00	-	-	1924.2	-	-

Na_3P	1.00	-	-	804.5	-	-
Li_3P	1.00	-	-	1552.3	-	-
AlP	3.00	-	-	1387.3	-	-
Si_3P_4	4.00	-	-	1545.1	-	-
K_3P	1.00	-	-	542.3	-	-
Ca_3P_2	2.00	-	-	882.7	-	-
ScP	3.00	-	-	1058.9	-	-
TiP	3.00	-	-	1019.8	-	-
(VP)	3.00	-	-	981.6	-	-
CrP	3.00	-	-	969.1	-	-
MnP	3.00	-	-	935.9	-	-
Mn_2P	1.50	-	-	570.9	-	-
FeP	3.00	-	-	926.1	-	-
Fe_2P	1.50	-	-	563.6	-	-
Fe_3P	1.00	-	-	405.0	-	-
Co_2P	1.50	-	-	540.2	-	-
Ni_2P	1.50	-	-	542.0	-	-
Ni_3P	1.00	-	-	388.3	-	-
Ni_5P_2	1.20	-	-	452.5	-	-
CuP_2	6.00	-	-	1281.4	-	-
Cu_3P	1.00	-	-	362.8	-	-
Zn_3P_2	2.00	-	-	623.0	-	-
GaP	3.00	-	-	798.5	-	-
GeP	3.00	-	-	776.0	-	-
Ge_3P_4	4.00	-	-	940.9	-	-
As_3P_5	5.00	-	-	1059.0	-	-
$Se(P)_2$	6.00	-	-	1141.2	-	-
YP	3.00	-	-	670.7	-	-
ZrP_2	6.00	-	-	1049.9	-	-
NbP	3.00	-	-	649.0	-	-
MoP	3.00	-	-	633.5	-	-
RuP	3.00	-	-	608.9	-	-
AgP_2	6.00	-	-	947.0	-	-
AgP_3	9.00	-	-	1201.3	-	-
LaP	3.00	-	-	473.3	-	-
Ce_3P_4	4.00	-	-	590.9	-	-
WP_2	6.00	-	-	654.3	-	-

Cl						
$BeCl_2$	2.00	-146.2	0.758	670.7	389.7	724.6
PCl_5	5.00	-1174.6	2.435	643.5	1212.9	2432.7
NaCl	1.00	88.2	-0.914	458.6	-347.0	-722.2
LiCl	1.00	88.5	-0.917	632.2	-450.7	-974.5
$AlCl_3$	3.00	-258.9	0.894	603.0	423.5	962.2
KCl	1.00	112.6	-1.167	359.5	-360.7	-703.0
$CaCl_2$	2.00	157.0	-0.814	483.0	-322.4	-664.8
$ScCl_3$	3.00	-61.8	0.214	531.4	91.4	204.3
$TiCl_2$	2.00	-127.4	0.660	451.3	247.3	681.5
$TiCl_3$	3.00	-234.2	0.809	521.3	341.2	819.4
VCl_2	2.00	-185.8	0.963	439.9	353.1	998.1
VCl_3	3.00	-376.4	1.300	511.2	539.6	1424.3
$CrCl_2$	2.00	-235.8	1.222	436.1	445.0	1156.0
$CrCl_3$	3.00	-401.6	1.387	507.7	572.6	1423.8
$MnCl_2$	2.00	-151.3	0.784	425.9	279.9	747.1
$FeCl_2$	2.00	-289.5	1.500	422.9	532.4	1490.1
$FeCl_3$	3.00	-553.7	1.913	495.7	774.2	1999.8
$CoCl_2$	2.00	-322.0	1.669	412.8	580.3	1699.6
$NiCl_2$	2.00	-332.8	1.725	413.6	600.7	1815.9
CuCl	1.00	-176.0	1.824	270.7	439.8	1581.9
$CuCl_2$	2.00	-416.1	2.156	398.7	728.1	2159.3
$ZnCl_2$	2.00	-222.4	1.153	393.3	384.7	1014.9
$GaCl_3$	3.00	-432.9	1.496	456.6	565.8	1303.3
$AsCl_5$	5.00	-	-	531.4	-	-
$SeCl_4$	4.00	-	-	485.6	-	-
YCl_3	3.00	40.0	-0.138	411.8	-48.0	-116.1
$ZrCl_2$	2.00	-205.8	1.066	330.6	306.6	875.6
$ZrCl_3$	3.00	-241.7	0.835	406.9	286.9	782.9
$ZrCl_4$	4.00	-293.7	0.761	460.0	289.7	733.7
$NbCl_5$	5.00	-796.3	1.651	496.0	668.4	1673.9
$NbCl_4$	4.00	-578.1	1.498	456.7	566.7	1584.8
$MoCl_4$	4.00	-781.6	2.025	450.9	758.2	-
$MoCl_5$	5.00	-1056.5	2.190	490.5	878.7	2289.1
$MoCl_6$	6.00	-1384.4	2.391	521.0	1007.8	-

$RuCl_3$	3.00	-728.0	2.515	387.6	829.1	2300.8
AgCl	1.00	-186.1	1.929	187.0	332.5	1577.5
$SnCl_2$	2.00	-305.6	1.584	282.7	396.8	1369.3
$LaCl_3$	3.00	-	-	327.8	-	-
$CeCl_3$	3.00	97.1	-0.335	326.2	-95.3	-324.7
WCl_2	2.00	-371.8	1.927	210.4	370.1	1698.4
WCl_4	4.00	-823.6	2.134	329.2	611.3	2323.6
WCl_5	5.00	-1077.5	2.234	371.1	709.5	2337.8
WCl_6	6.00	-1319.4	2.279	405.5	780.7	2370.5
BO_2^-						
$NaBO_2$	1.00	-	-	407.3	-	-
$LiBO_2$	1.00	-	-	538.7	-	-
$Al\ (BO_2)_3$	3.00	-	-	517.4	-	-
KBO_2	1.00	-	-	327.2	-	-
$Sc(BO_2)_3$	3.00	-	-	463.7	-	-
$Ti\ (BO_2)_4$	4.00	-	-	489.3	-	-
$V(BO_2)_5$	5.00	-	-	505.7	-	-
$Cr(BO_2)_6$	6.00	-	-	520.6	-	-
$Mn\ (BO_2)_3$	3.00	-	-	438.5	-	-
$Fe\ (BO_2)_2$	2.00	-	-	378.9	-	-
$Co\ (BO_2)_3$	3.00	-	-	429.1	-	-
$Ni(BO_2)_2$	2.00	-	-	371.4	-	-
$Cu(BO_2)_2$	2.00	-	-	359.3	-	-
$Zn(BO_2)_2$	2.00	-	-	355.0	-	-
$Ga(BO_2)_3$	3.00	-	-	405.8	-	-
$Ge(BO_2)_4$	4.00	-	-	439.6	-	-
$Y\ (BO_2)_3$	3.00	-	-	369.9	-	-
$Zr\ (BO_2)_4$	4.00	-	-	408.5	-	-
$Nb\ BO_2$	1.00	-	-	197.5	-	-
$MoBO_2$	1.00	-	-	193.2	-	-
$Ru(BO_2)_2$	2.00	-	-	287.1	-	-
$Ag\ BO_2$	1.00	-	-	177.9	-	-
$La\ (BO_2)_3$	3.00	-	-	300.8	-	-
$Ce(BO_2)_4$	4.00	-	-	344.3	-	-
$W\ (BO_2)_6$	6.00	-	-	364.9	-	-

$Be_3(BO_3)_2$	2.00	-	-	1111.8	-	-
$Ca_3(BO_3)_2$	2.00	-	-	676.1	-	-
CO_3^{2-}						
Be CO_3	2.00	-	-	776.6	-	-
$B_2(CO_3)_3$	3.00	-	-	797.5	-	-
Na_2 CO_3	1.00	16.2	-0.167	505.7	-68.9	-161.0
Li_2CO_3	1.00	-	-	725.4	-	-
$Al_2(CO_3)_3$	3.00	-	-	687.2	-	-
K_2 CO_3	1.00	25.7	-0.266	387.8	-87.9	-192.1
$CaCO_3$	2.00	116.7	-0.605	535.6	-260.6	-645.9
Sc $_2(CO_3)_3$	3.00	-	-	595.7	-	-
Ti $(CO_3)_2$	4.00	-	-	638.6	-	-
$V_2(CO_3)_5$	5.00	-	-	666.8	-	-
Cr $(CO_3)_3$	6.00	-	-	693.1	-	-
$MnCO_3$	2.00	-195.4	1.013	466.3	389.8	1204.8
$Fe_2(CO_3)_3$	3.00	-	-	551.2	-	-
$FeCO_3$	2.00	-345.4	1.790	450.7	669.8	2173.5
$CoCO_3$	2.00	-375.3	1.945	450.7	727.8	2464.4
Ni CO_3	2.00	-394.2	2.043	451.6	765.7	2668.9
$CuCO_3$	2.00	-	-	433.8	-	-
Zn CO_3	2.00	-280.5	1.454	427.5	520.5	1843.7
$Ga_2(CO_3)_3$	3.00	-	-	503.4	-	-
$Ge(CO_3)_2$	4.00	-	-	556.5	-	-
$Y_2(CO_3)_3$	3.00	-	-	449.4	-	-
$ZrCO_3$	2.00	-	-	354.4	-	-
Nb_2 CO_3	1.00	-	-	218.1	-	-
Mo_2CO_3	1.00	-	-	212.8	-	-
Ru_2CO_3	1.00	-	-	204.5	-	-
Ag_2 CO_3	1.00	-287.7	2.981	194.4	532.6	2692.2
La $_2(CO_3)_3$	3.00	-	-	351.2	-	-
$Ce_2(CO_3)_3$	3.00	-	-	349.4	-	-
W $(CO_3)_3$	6.00	-	-	441.9	-	-
PO_4^{3-}						
$Be_{3(}PO_{4)2}$	2.00	-	-	741.1	-	-

Na_3PO_4	1.00	6.5	-0.067	490.4	-27.0	-63.2
Li_3PO_4(Δ H=-698.6 kJ mol^{-1})	1.00	-356.9	3.699	694.4	1953.6	4040.8
Al PO_4	3.00	-151.4	0.523	659.3	265.5	612.9
K_3 PO_4	1.00	-	-	378.8	-	-
$Ca_3(PO_4)_2$	2.00	115.3	-0.598	518.4	-250.9	-682.9
Sc PO_4	3.00	-	-	574.6	-	-
Ti $_3(PO_4)_4$	4.00	-	-	614.4	-	-
V_3 $(PO_4)_5$	5.00	-	-	640.5	-	-
$CrPO_4$	3.00	-	-	547.1	-	-
Mn PO_4	3.00	-	-	536.4	-	-
Mn_3(PO_4)2	2.00	-	-	453.3	-	-
Fe PO_4	3.00	-581.8	2.010	533.1	863.0	2198.0
$Co_3(PO_4)_2$	2.00	-	-	438.5	-	-
$Ni_3(PO_4)_2$	2.00	-	-	439.3	-	-
$Cu_3(PO_4)_2$	2.00	-	-	422.5	-	-
$Zn_3(PO_4)_2$	2.00	-291.7	1.512	416.5	529.5	1755.2
Ga PO_4	3.00	-	-	488.2	-	-
$Ge_3(PO_4)_4$	4.00	-	-	538.0	-	-
Y PO_4	3.00	-	-	437.3	-	-
Zr $_3(PO_4)_2$	2.00	-	-	346.9	-	-
Nb_3 PO_4	1.00	-	-	215.2	-	-
Mo_3PO_4	1.00	-	-	210.0	-	-
Ru_3 PO_4	1.00	-	-	201.9	-	-
Ag_3 PO_4	1.00	-	-	192.1	-	-
La PO_4	3.00	-	-	343.8	-	-
$CePO_4$	3.00	-	-	342.0	-	-
W $(PO_4)_2$	6.00	-	-	430.2	-	-
SO_4^{2-}						
Be SO_4	2.00	-81.2	0.421	510.1	174.3	402.7
Na_2 SO_4	1.00	49.8	-0.516	377.4	-166.3	-415.5
Li_2 SO_4	1.00	75.6	-0.783	487.5	-312.6	-758.8
Al_2($SO_4)_3$	3.00	-2.4	0.008	470.0	3.2	-
$AlK(SO_4)_2$	4.00	-101.1	0.262	415.2	91.5	-

$K_2 SO_4$	1.00	75.4	-0.781	307.6	-211.0	-526.9
$CaSO_4$	2.00	138.5	-0.718	393.7	-239.8	-641.4
$Sc_2(SO_4)_3$	3.00	-	-	425.3	-	-
$Ti(SO_4)_2$	4.00	-	-	446.7	-	-
$V_2(SO_4)_5$	5.00	-	-	460.3	-	-
$Cr_2(SO_4)_3$	3.00	-447.3	1.545	410.0	534.3	1475.2
$MnSO_4$	2.00	-213.2	1.105	355.0	337.8	979.7
$FeSO_4$	2.00	-349.8	1.813	352.9	551.4	1747.5
$Fe_2(SO_4)_3$	3.00	-624.6	2.158	402.1	733.9	2029.7
$Co SO_4$	2.00	-388.2	2.012	345.8	601.4	1933.8
$Ni SO_4$	2.00	-410.9	2.129	346.4	637.4	2170.9
$CuSO_4$	2.00	-508.4	2.635	335.8	767.9	2421.5
$Zn SO_4$	2.00	-299.1	1.550	332.0	447.3	1471.2
$Y_2(SO_4)_3$	3.00	-	-	345.1	-	-
$Zr(SO_4)_2$	4.00	-	-	378.3	-	-
Nb_2SO_4	1.00	-	-	190.2	-	-
Mo_2SO_4	1.00	-	-	186.2	-	-
Ru_2SO_4	1.00	-	-	179.8	-	-
$Ag_2 SO_4$	1.00	-276.1	2.862	171.9	456.4	2154.5
$La_2(SO_4)_3$	3.00	-	-	284.1	-	-
$Ce_2(SO_4)_3$	3.00	45.6	-0.157	282.9	-39.5	-
$W(SO_4)_3$	6.00	-	-	340.7	-	-

Al						
M_aX_b	n	Δ_rG (kJ mol^{-1})	EMF (V)	Capacity (m A h g^{-1})	Cal. Energy density (W h kg^{-1})	Cal. Energy density (W h L^{-1})
F						
BeF_2	2.00	25.3	-0.131	1140.3	-108.3	-242.3
NaF	1.00	69.3	-0.718	638.3	-377.4	-1043.9
MgF_2	2.00	117.0	-0.606	860.4	-404.9	-1229.2
LiF	1.00	110.7	-1.147	1033.2	-880.0	-2628.3
KF	1.00	60.8	-0.630	461.3	-251.6	-630.9
CaF_2	2.00	221.5	-1.148	686.6	-640.6	-1971.8

ScF_3	3.00	108.7	-0.376	788.7	-234.3	-593.1
TiF_3	3.00	-69.1	0.239	766.8	145.6	424.9
TiF_4	4.00	-349.1	0.905	865.5	606.8	1684.2
VF_3	3.00	-204.4	0.706	744.9	420.9	1349.4
CrF_3	3.00	-327.7	1.132	737.7	669.4	2353.8
MnF_2	2.00	-147.0	0.762	576.8	368.0	1360.4
MnF_3	3.00	-431.3	1.490	718.3	862.4	2879.5
FeF_2	2.00	-285.5	1.479	571.2	709.1	2678.8
FeF_3	3.00	-459.1	1.586	712.5	912.1	3258.0
CoF_2	2.00	-306.9	1.590	553.0	741.8	3002.5
CoF_3	3.00	-712.1	2.460	693.6	1384.1	4962.0
NiF_2	2.00	-350.0	1.814	554.4	847.7	3570.1
CuF	1.00	-217.0	2.249	324.7	658.6	4031.4
CuF_2	2.00	-462.1	2.395	527.9	1073.8	4185.9
ZnF_2	2.00	-240.8	1.248	518.5	551.0	2409.5
GaF_3	3.00	-345.8	1.195	634.5	625.0	2505.7
RbF	1.00	51.5	-0.534	256.6	-126.1	-437.4
YF_3	3.00	213.6	-0.738	551.1	-343.2	-1277.1
ZrF_2	2.00	-41.1	0.213	414.8	77.5	-
ZrF_3	3.00	-105.5	0.000	542.5	167.3	654.7
ZrF_4	4.00	-98.2	0.255	641.1	134.3	534.4
NbF_5	5.00	-686.2	1.422	713.2	818.5	2210.3
RuF_3	3.00	-	-	508.7	-	-
RuF_5	5.00	-1603.9	3.325	683.5	1848.4	6658.1
AgF	1.00	-290.0	3.006	211.3	593.0	3221.6
SnF_2	2.00	-352.6	1.827	342.1	560.7	2391.9
LaF_3	3.00	192.7	-0.666	410.4	-240.1	-1239.2
CeF_3	3.00	124.9	-0.432	407.9	-154.8	-826.1
O						
BeO-α	2.00	52.7	-0.273	2143.1	-340.3	-977.7
B_2O_3	3.00	-194.0	0.670	2309.7	872.0	2279.7
Na_2O	1.00	-76.0	0.787	864.9	527.7	1242.6
MgO microcrystal	2.00	41.9	-0.217	1329.9	-199.6	-662.8
Li_2O	1.00	16.9	-0.175	1793.9	-196.0	-436.4
SiO_2 quartz	4.00	-198.5	0.514	1784.3	574.1	1510.7

SiO_2 high cristobalite	4.00	-201.2	0.521	1784.3	581.9	1431.3
P_4O_{10}	5.00	-637.7	1.322	1888.2	1527.9	3545.6
K_2O	1.00	-102.7	1.064	569.1	508.4	1220.2
CaO	2.00	75.9	-0.393	955.9	-284.6	-898.9
Sc_2O_3	3.00	118.6	-0.410	1166.0	-343.3	-1183.4
TiO	2.00	-32.4	0.168	839.3	110.0	460.5
Ti_2O_3	3.00	-74.0	0.256	1118.8	208.1	790.8
Ti_3O_5	3.33	-106.6	0.331	1198.6	283.3	1032.4
TiO_2-R	4.00	-165.8	0.430	1342.3	397.5	1418.4
TiO_2	4.00	-166.0	0.430	1342.3	398.2	1420.7
TiO_2-A	4.00	-171.9	0.445	1342.3	412.3	1413.2
VO	2.00	-123.2	0.639	800.7	403.0	2239.2
V_2O_3	3.00	-221.5	0.765	1072.9	603.6	2424.7
VO_2	4.00	263.6	-0.683	1292.6	-615.8	-2258.0
V_3O_5	3.33	-278.0	0.865	1151.2	717.9	-
V_2O_5	5.00	-608.8	1.262	1473.6	1244.3	3862.0
CrO_2	4.00	-509.9	1.321	1276.3	1180.7	4645.7
Cr_2O_3	3.00	-262.1	0.905	1058.0	707.0	2966.1
Cr_3O_4 (Δ H=-1513 kJ mol^{-1})	2.67	-192.9	0.750	974.7	550.6	2564.1
CrO_3	6.00	-1069.7	1.848	1608.2	1930.0	5212.4
MnO_2	4.00	-589.7	1.528	1233.1	1332.8	5383.8
Mn_2O_3	3.00	-350.6	1.211	1018.6	919.4	3778.5
MnO	2.00	-164.5	0.853	755.6	513.9	2300.3
Mn_3O_4	2.67	-275.5	1.071	937.1	763.3	3106.5
FeO	2.00	-276.0	1.430	746.1	853.5	4115.3
Fe_2O_3 hematite	3.00	-420.0	1.451	1007.0	1092.2	4631.1
Fe_3O_4 magnetite	2.67	-364.8	1.418	926.1	1001.6	4256.5
CoO	2.00	-313.2	1.623	715.3	936.4	4756.4
Co_3O_4	2.67	-445.2	1.730	890.4	1186.3	5618.3
NiO	2.00	-315.7	1.636	717.6	946.3	5256.9
Ni_2O_3	3.00	-	-	972.3	-	-
CuO	2.00	-397.7	2.061	673.9	1132.7	5735.2
Cu_2O	1.00	-190.7	1.977	374.6	657.8	3473.1

ZnO	2.00	-206.9	1.072	658.6	578.4	2712.4
Ga_2O_3	3.00	-292.0	1.009	857.9	672.0	3167.5
GeO	2.00	-290.2	1.504	604.7	756.1	-
GeO_2	4.00	-533.4	1.382	1024.5	1053.8	3906.1
As_4O_6 octahedral	3.00	-503.0	1.738	812.8	1109.8	3879.3
As_2O_5	5.00	-927.4	1.922	1166.1	1611.2	5957.1
SeO_2	4.00	-883.4	2.289	966.2	1670.0	5926.4
Y_2O_3	3.00	117.2	-0.405	712.1	-232.7	-1003.5
ZrO_2	4.00	-12.0	0.031	870.0	21.0	95.6
NbO	2.00	-135.5	0.702	492.2	296.6	1744.3
NbO_2	4.00	-314.3	0.814	858.3	542.8	2532.1
Nb_2O_5	5.00	-435.7	0.903	1008.3	680.3	2609.5
MoO_2	4.00	-521.8	1.352	837.9	884.4	4380.9
MoO_3	6.00	-914.3	1.579	1117.2	1283.3	5019.4
RuO_2	4.00	-774.8	2.008	805.6	1273.2	6686.5
RuO_4	8.00	-1957.5	2.536	1298.9	2294.1	7079.9
AgO	2.00	-541.3	2.805	432.7	1059.9	6488.1
Ag_2O	1.00	-258.1	2.675	231.3	574.2	3691.6
Ag_2O_3	3.00	-851.8	2.943	609.7	1489.6	-
La_2O_3	3.00	61.8	-0.213	493.6	-90.4	-490.1
CeO_2	4.00	-30.2	0.078	622.9	40.4	226.1
Ce_2O_3	3.00	62.0	-0.214	489.9	-90.1	-472.1
WO_2	4.00	-520.9	1.350	496.7	574.7	4345.6
WO_3	6.00	-818.3	1.413	693.6	795.3	4356.8
S						
BeS	2.00	19.7	-0.102	1304.9	-92.5	-227.0
B_2S_3	3.00	-196.2	0.678	1364.8	634.5	1220.9
Na_2S	1.00	68.2	-0.707	686.8	-394.7	-778.3
MgS	2.00	128.5	-0.666	950.9	-479.9	-1288.7
Li_2S	1.00	112.8	-1.169	1166.6	-980.4	-2131.9
SiS_2	4.00	-214.1	0.555	1162.5	463.9	1016.1
P_4S_3	1.50	-120.3	0.831	730.6	487.5	1040.7
P_4S_7	3.50	-298.5	0.884	1077.1	699.4	1612.9
P_2S_5	5.00	-463.7	0.961	1205.8	825.1	1804.3
K_2S	1.00	75.3	-0.781	486.1	-326.3	-597.7

CaS	2.00	264.1	-1.368	743.0	-813.8	-2125.4
Sc_2S_3	3.00	-	-	864.1	-	-
TiS_2	4.00	-24.5	0.063	957.2	46.0	146.1
TiS	2.00	56.7	-0.294	670.6	-161.0	-574.8
Ti_2S_3	3.00	-	-	837.8	-	-
VS	2.00	-	-	645.8	-	-
V_2S_3	3.00	-	-	811.8	-	-
VS_2	4.00	-	-	931.6	-	-
V_2S_5	5.00	-	-	1022.1	-	-
CrS	2.00	-38.9	0.202	637.7	105.9	-
Cr_2S_3	3.00	-236.1	0.816	803.3	516.0	1794.8
MnS	2.00	5.1	-0.026	616.1	-13.4	-45.0
MnS_2	4.00	-201.7	0.523	900.4	361.3	-
FeS	2.00	-112.9	0.585	609.7	296.2	1236.9
FeS_2(marcasite)	4.00	-270.6	0.701	893.6	481.9	2019.6
FeS_2(pyrite)	4.00	-259.8	0.673	893.6	462.7	1939.0
CoS	2.00	-	-	589.0	-	-
Co_2S_3	3.00	-	-	751.2	-	-
CoS_2	4.00	-281.0	0.728	871.1	490.8	1861.5
Co_3S_4	2.67	-122.1	0.475	702.8	270.0	-
NiS	2.00	-133.8	0.694	590.6	341.9	1605.3
Ni_3S_4	2.67	-187.1	0.727	704.5	414.4	1724.4
Ni_3S_2	1.33	-72.2	0.561	446.3	217.9	-
NiS_2	4.00	-302.0	0.782	872.8	528.2	-
CuS	2.00	-159.7	0.828	560.6	390.6	1659.1
Cu_2S	1.00	-63.6	0.659	336.8	199.4	1006.7
ZnS	2.00	-12.0	0.062	550.0	29.0	109.1
Ga_2S_3	3.00	-67.1	0.232	682.4	128.8	445.9
GaS	2.00	-8.6	0.045	526.6	20.1	72.7
GeS	2.00	-141.8	0.735	511.9	321.1	1223.7
GeS_2	4.00	-272.1	0.705	783.8	437.5	1286.3
As_2S_3	3.00	-235.7	0.814	653.6	436.5	1437.7
Se_2S_6	6.00	-	-	918.1	-	-
Se_4S_4	2.00	-	-	482.8	-	-
RuS_2	4.00	-	-	648.9	-	-
Y_2S_3	3.00	-	-	586.9	-	-

ZrS_2	4.00	143.3	-0.371	690.1	-208.1	-744.9
NbS_2	4.00	-	-	682.7	-	-
MoS_2	4.00	-200.8	0.520	669.7	284.5	1240.7
Mo_2S_3	3.00	-180.7	0.624	558.2	293.5	1460.9
Ag_2S(argentite)	1.00	-86.3	0.895	216.3	180.5	1171.8
LaS	2.00	238.2	-1.234	313.5	-350.1	-1781.6
La_2S_3	3.00	284.2	-0.982	430.0	-368.9	-1639.3
CeS	2.00	238.2	-1.234	311.3	-347.9	-1845.9
WS_2	4.00	-176.8	0.458	432.3	172.9	1068.8
N						
Be_3N_2	2.00	-13.7	0.071	2921.1	104.7	283.4
BN	3.00	-58.6	0.202	3239.7	314.2	761.7
(CN)	3.00	-	-	3090.4	-	-
Na_3N	1.00	-	-	969.0	-	-
Mg_3N2	2.00	-57.7	0.299	1593.3	310.4	840.4
Li_3N	1.00	-52.8	0.547	2308.5	711.8	2127.0
Si_3N_4	4.00	-168.5	0.437	2292.6	565.6	1667.4
K_3N	1.00	-	-	612.4	-	-
Ca_3N_2	2.00	-68.7	0.356	1084.7	283.0	757.9
ScN	3.00	-3.2	0.011	1363.6	10.5	-
TiN	3.00	-43.2	0.149	1299.5	135.1	548.9
VN	3.00	-95.9	0.331	1238.0	289.8	1294.6
CrN	3.00	-194.0	0.670	1218.2	579.5	2545.2
Cr_2N	1.50	-92.4	0.638	681.4	354.1	1877.7
Mn_4N	0.75	-45.5	0.629	344.0	193.9	-
Mn_5N_2	1.20	-83.8	0.724	531.2	326.3	-
Fe_2N	1.50	-	-	639.7	-	-
Fe_4N	0.75	-70.8	0.979	338.7	297.6	-
Co_3N	1.00	-84.2	0.873	421.4	322.2	1763.3
NiN	3.00	-	-	1106.0	-	-
Cu_3N	1.00	-	-	392.9	-	-
Zn_3N_2	2.00	-204.4	1.059	717.3	612.5	3041.6
GaN	3.00	-209.3	0.723	960.3	525.0	2451.4
Ge_3N_4	4.00	-	-	1174.0	-	-
As_3N_5	5.00	-	-	1363.7	-	-
SeN_2	6.00	-	-	1503.3	-	-

YN	3.00	-18.4	0.064	781.3	39.4	180.5
ZrN	3.00	49.7	-0.172	764.1	-104.4	-556.1
NbN	3.00	-81.1	0.280	752.1	168.3	996.4
MoN	3.00	-	-	731.3	-	-
RuN	3.00	-	-	698.7	-	-
Ag_3N	1.00	-	-	238.2	-	-
LaN	3.00	-16.0	0.055	525.8	24.7	135.6
CeN	3.00	8.0	-0.027	521.7	-12.2	-74.8
WN_2	6.00	-	-	759.1	-	-
NaN_3	1.00	-	-	179.8	-	-
KN_3	1.00	-	-	162.3	-	-
AgN_3	1.00	-	-	114.6	-	-
P						
Be_3P_2	2.00	-	-	1807.2	-	-
BP	3.00	-84.9	0.293	1924.2	342.8	-
Na_3P	1.00	-	-	804.5	-	-
Mg_3P_2	2.00	-	-	1192.4	-	-
Li_3P	1.00	-	-	1552.3	-	-
Si_3P_4	4.00	-	-	1545.1	-	-
K_3P	1.00	-	-	542.3	-	-
Ca_3P_2	2.00	55.3	-0.287	882.7	-195.2	-498.0
ScP	3.00	-	-	1058.9	-	-
TiP	3.00	-	-	1019.8	-	-
(VP)	3.00	-	-	981.6	-	-
CrP	3.00	-	-	969.1	-	-
MnP	3.00	-47.2	0.163	935.9	116.2	511.6
Mn_2P	1.50	4.5	-0.031	570.9	-15.0	-75.4
FeP	3.00	-	-	926.1	-	-
Fe_2P	1.50	-	-	563.6	-	-
Fe_3P	1.00	-	-	405.0	-	-
Co_2P	1.50	11.5	-0.080	540.2	-36.4	-192.6
Ni_2P	1.50	9.6	-0.067	542.0	-30.5	-177.0
Ni_3P	1.00	18.2	-0.188	388.3	-64.7	-
Ni_5P_2	1.20	21.1	-0.182	452.5	-71.6	-
CuP_2	6.00	-204.8	0.354	1281.4	316.9	1140.9
Cu_3P	1.00	-4.2	0.044	362.8	14.2	81.9
Zn_3P_2	2.00	-	-	623.0	-	-
GaP	3.00	-66.5	0.230	798.5	144.8	538.5

GeP	3.00	-140.9	0.487	776.0	299.6	-
Ge_3P_4	4.00	-	-	940.9	-	-
As_3P_5	5.00	-	-	1059.0	-	-
$Se(P)_2$	6.00	-	-	1141.2	-	-
YP	3.00	-	-	670.7	-	-
ZrP_2	6.00	-	-	1049.9	-	-
NbP	3.00	-	-	649.0	-	-
MoP	3.00	-	-	633.5	-	-
RuP	3.00	-	-	608.9	-	-
AgP_2	6.00	-914.8	1.580	947.0	766.1	-
AgP_3	9.00	-1369.2	1.577	1201.3	857.3	-
LaP	3.00	-	-	473.3	-	-
Ce_3P_4	4.00	-	-	590.9	-	-
WP_2	6.00	-	-	654.3	-	-
Cl						
$BeCl_2$	2.00	26.4	-0.137	670.7	-74.9	-150.5
PCl_5	5.00	-743.1	1.540	643.5	815.2	1782.5
NaCl	1.00	174.5	-1.809	458.6	-718.8	-1601.8
$MgCl_2$	2.00	172.6	-0.894	563.0	-423.5	-1007.1
LiCl	1.00	174.8	-1.812	632.2	-944.9	-2377.5
KCl	1.00	198.9	-2.061	359.5	-661.3	-1353.2
$CaCl_2$	2.00	329.6	-1.708	483.0	-709.9	-1571.0
$ScCl_3$	3.00	197.1	-0.681	531.4	-307.1	-749.6
$TiCl_2$	2.00	45.2	-0.234	451.3	-91.8	-281.5
$TiCl_3$	3.00	24.7	-0.085	521.3	-37.9	-100.3
VCl_2	2.00	-13.2	0.068	439.9	26.2	82.6
VCl_3	3.00	-117.5	0.406	511.2	177.1	522.9
$CrCl_2$	2.00	-63.2	0.328	436.1	124.6	355.9
$CrCl_3$	3.00	-142.7	0.493	507.7	213.9	588.5
$MnCl_2$	2.00	21.3	-0.110	425.9	-41.1	-120.9
$FeCl_2$	2.00	-116.9	0.606	422.9	224.4	696.2
$FeCl_3$	3.00	-294.8	1.018	495.7	432.8	1242.3
$CoCl_2$	2.00	-149.4	0.774	412.8	280.7	916.1
$NiCl_2$	2.00	-160.2	0.830	413.6	301.5	1021.1
CuCl	1.00	-89.7	0.930	270.7	230.7	914.7
$CuCl_2$	2.00	-243.5	1.262	398.7	443.7	1464.0

$ZnCl_2$	2.00	-49.8	0.258	393.3	89.7	258.4
$GaCl_3$	3.00	-174.0	0.601	456.6	238.0	594.7
$AsCl_5$	5.00	-	-	531.4	-	-
$SeCl_4$	4.00	-	-	485.6	-	-
YCl_3	3.00	298.9	-1.033	411.8	-373.6	-979.2
$ZrCl_2$	2.00	-33.2	0.172	330.6	51.2	159.1
$ZrCl_3$	3.00	17.2	-0.059	406.9	-21.3	-63.9
$ZrCl_4$	4.00	51.5	-0.133	460.0	-53.2	-148.2
$NbCl_5$	5.00	-364.8	0.756	496.0	321.5	890.2
$NbCl_4$	4.00	-232.9	0.603	456.7	239.0	746.4
$MoCl_4$	4.00	-436.4	1.131	450.9	442.9	-
$MoCl_5$	5.00	-625.0	1.296	490.5	545.6	1579.9
$MoCl_6$	6.00	-866.6	1.497	521.0	663.8	-
$RuCl_3$	3.00	-469.1	1.621	387.6	555.9	1694.4
AgCl	1.00	-99.8	1.034	187.0	182.0	952.5
$SnCl_2$	2.00	-133.0	0.689	282.7	177.9	675.8
$LaCl_3$	3.00	-	-	327.8	-	-
$CeCl_3$	3.00	356.0	-1.230	326.2	-361.6	-1372.1
WCl_2	2.00	-199.2	1.032	210.4	202.9	1034.7
WCl_4	4.00	-478.4	1.240	329.2	367.5	1585.8
WCl_5	5.00	-646.0	1.339	371.1	441.9	1635.6
WCl_6	6.00	-801.6	1.385	405.5	494.2	1678.9
BO_2-						
$NaBO_2$	1.00	-	-	407.3	-	-
$Mg(BO_2)_2$	2.00	-	-	487.6	-	-
$LiBO_2$	1.00	-	-	538.7	-	-
KBO_2	1.00	-	-	327.2	-	-
$Sc(BO_2)_3$	3.00	-	-	463.7	-	-
$Ti\ (BO_2)_4$	4.00	-	-	489.3	-	-
$V(BO_2)_5$	5.00	-	-	505.7	-	-
$Cr(BO_2)_6$	6.00	-	-	520.6	-	-
$Mn\ (BO_2)_3$	3.00	-	-	438.5	-	-
$Fe\ (BO_2)_2$	2.00	-	-	378.9	-	-
$Co\ (BO_2)_3$	3.00	-	-	429.1	-	-
$Ni(BO_2)_2$	2.00	-	-	371.4	-	-

$Cu(BO_2)_2$	2.00	-	-	359.3	-	-
$Zn(BO_2)_2$	2.00	-	-	355.0	-	-
$Ga(BO_2)_3$	3.00	-	-	405.8	-	-
$Ge(BO_2)_4$	4.00	-	-	439.6	-	-
$Y\ (BO_2)_3$	3.00	-	-	369.9	-	-
$Zr\ (BO_2)_4$	4.00	-	-	408.5	-	-
$Nb\ BO_2$	1.00	-	-	197.5	-	-
$MoBO_2$	1.00	-	-	193.2	-	-
$Ru(BO_2)_2$	2.00	-	-	287.1	-	-
$Ag\ BO_2$	1.00	-	-	177.9	-	-
$La\ (BO_2)_3$	3.00	-	-	300.8	-	-
$Ce(BO_2)_4$	4.00	-	-	344.3	-	-
$W\ (BO_2)_6$	6.00	-	-	364.9	-	-
$Be_3(BO_3)_2$	2.00	-	-	1111.8	-	-
$Ca_3(BO_3)_2$	2.00	-	-	676.1	-	-
CO_3^{2-}						
$Be\ CO_3$	2.00	-	-	776.6	-	-
$B_2(CO_3)_3$	3.00	-	-	797.5	-	-
$Na_2\ CO_3$	1.00	-	-	505.7	-	-
$Mg\ CO_3$	2.00	-	-	635.8	-	-
Li_2CO_3	1.00	-	-	725.4	-	-
$K_2\ CO_3$	1.00	-	-	387.8	-	-
$CaCO_3$	2.00	-	-	535.6	-	-
$Sc\ _2(CO_3)_3$	3.00	-	-	595.7	-	-
$Ti\ (CO_3)_2$	4.00	-	-	638.6	-	-
$V_2(CO_3)_5$	5.00	-	-	666.8	-	-
$Cr\ (CO_3)_3$	6.00	-	-	693.1	-	-
$MnCO_3$	2.00	-	-	466.3	-	-
$Fe_2(CO_3)_3$	3.00	-	-	551.2	-	-
$FeCO_3$	2.00	-	-	450.7	-	-
$CoCO_3$	2.00	-	-	450.7	-	-
$Ni\ CO_3$	2.00	-	-	451.6	-	-
$CuCO_3$	2.00	-	-	433.8	-	-
$Zn\ CO_3$	2.00	-	-	427.5	-	-

$Ga_2(CO_3)_3$	3.00	-	-	503.4	-	-
$Ge(CO_3)_2$	4.00	-	-	556.5	-	-
$Y_2(CO_3)_3$	3.00	-	-	449.4	-	-
$ZrCO_3$	2.00	-	-	354.4	-	-
$Nb_2\ CO_3$	1.00	-	-	218.1	-	-
Mo_2CO_3	1.00	-	-	212.8	-	-
Ru_2CO_3	1.00	-	-	204.5	-	-
$Ag_2\ CO_3$	1.00	-	-	194.4	-	-
$La\ _2(CO_3)_3$	3.00	-	-	351.2	-	-
$Ce_2(CO_3)_3$	3.00	-	-	349.4	-	-
$W\ (CO_3)_3$	6.00	-	-	441.9	-	-
PO_4^{3-}						
$Be_3(PO_4)_2$	2.00	-	-	741.1	-	-
Na_3PO_4	1.00	57.0	-0.590	490.4	-248.6	-636.8
$Mg_3(PO_4)_2$	2.00	100.9	-0.523	611.8	-265.5	-603.2
Li_3PO_4(ΔH=-698.6 kJ mol^{-1})	1.00	-306.5	3.176	694.4	1788.7	4625.1
$K_3\ PO_4$	1.00	-	-	378.8	-	-
$Ca_3(PO_4)_2$	2.00	216.3	-1.121	518.4	-494.9	-1517.6
$Sc\ PO_4$	3.00	-	-	574.6	-	-
$Ti\ _3(PO_4)_4$	4.00	-	-	614.4	-	-
$V_3\ (PO_4)_5$	5.00	-	-	640.5	-	-
$CrPO_4$	3.00	-	-	547.1	-	-
$Mn\ PO_4$	3.00	-	-	536.4	-	-
$Mn_3(\ PO_4\ )_2$	2.00	-	-	453.3	-	-
$Fe\ PO_4$	3.00	-430.4	1.487	533.1	672.4	1911.8
$Co_3(PO_4)_2$	2.00	-	-	438.5	-	-
$Ni_3(PO_4)_2$	2.00	-	-	439.3	-	-
$Cu_3(PO_4)_2$	2.00	-	-	422.5	-	-
$Zn_3(PO_4)_2$	2.00	-190.7	0.988	416.5	361.2	1364.4
$Ga\ PO_4$	3.00	-	-	488.2	-	-
$Ge_3(PO_4)_4$	4.00	-	-	538.0	-	-
$Y\ PO_4$	3.00	-	-	437.3	-	-
$Zr\ _3(PO_4)_2$	2.00	-	-	346.9	-	-

$Nb_3 PO_4$	1.00	-	-	215.2	-	-
Mo_3PO_4	1.00	-	-	210.0	-	-
$Ru_3 PO_4$	1.00	-	-	201.9	-	-
$Ag_3 PO_4$	1.00	-	-	192.1	-	-
$La PO_4$	3.00	-	-	343.8	-	-
$CePO_4$	3.00	-	-	342.0	-	-
$W (PO_4)_2$	6.00	-	-	430.2	-	-
SO_4^{2-}						
$Be SO_4$	2.00	-79.6	0.412	510.1	179.7	454.1
$Na_2 SO_4$	1.00	50.6	-0.524	377.4	-175.7	-474.3
$Mg SO_4$	2.00	1.6	-0.008	445.3	-3.2	-8.6
$Li_2 SO_4$	1.00	76.4	-0.791	487.5	-331.6	-
$AlK(SO_4)_2$	4.00	-97.9	0.254	415.2	92.4	-
$K_2 SO_4$	1.00	76.2	-0.790	307.6	-220.2	-586.6
$CaSO_4$	2.00	140.1	-0.726	393.7	-252.5	-739.1
$Sc_2(SO_4)_3$	3.00	-	-	425.3	-	-
$Ti (SO_4)_2$	4.00	-	-	446.7	-	-
$V_2(SO_4)_5$	5.00	-	-	460.3	-	-
$Cr_2(SO_4)_3$	3.00	-444.9	1.537	410.0	554.1	1687.5
$MnSO_4$	2.00	-211.6	1.096	355.0	347.8	1106.4
$FeSO_4$	2.00	-348.2	1.804	352.9	569.3	2003.5
$Fe_2(SO_4)_3$	3.00	-622.2	2.149	402.1	761.6	2320.3
$Co SO_4$	2.00	-386.6	2.003	345.8	620.8	2217.2
$Ni SO_4$	2.00	-409.3	2.121	346.4	658.2	2512.6
$CuSO_4$	2.00	-506.8	2.626	335.8	792.7	2760.7
$Zn SO_4$	2.00	-297.5	1.542	332.0	460.5	1681.5
$Y_2(SO_4)_3$	3.00	-	-	345.1	-	-
$Zr(SO_4)_2$	4.00	-	-	378.3	-	-
Nb_2SO_4	1.00	-	-	190.2	-	-
Mo_2SO_4	1.00	-	-	186.2	-	-
Ru_2SO_4	1.00	-	-	179.8	-	-
$Ag_2 SO_4$	1.00	-275.3	2.853	171.9	463.8	2394.7
$La_2(SO_4)_3$	3.00	-	-	284.1	-	-
$Ce_2(SO_4)_3$	3.00	48.0	-0.166	282.9	-42.8	-

$W(SO_4)_3$	6.00	-	-	340.7	-	-

Li					
X	Chemical Reaction	$\Delta_r G$ (kJ mol^{-1})	EMF (V)	Capacity (m A h g^{-1})	Cal. Energy density (W h kg^{-1})
F_2	$2Li+F_2=2LiF$	-1175.4	6.091	1410.7	6293.5
O_2	$4Li+O_2=2Li_2O$	-1122.4	2.908	3350.3	5216.9
N_2	$6Li+N_2=2Li_3N$	-257.2	0.444	5740.4	1025.6
S	$2Li+S=Li_2S$	-439.0	2.275	1671.6	2654.0
B	$3Li+B=Li_3B$	-	-	7436.6	-
Si	$4Li+Si=Li_4Si$	-	-	3817.1	-
P	$3Li+P=Li_3P$	-	-	2595.9	-
Cl_2	$2Li+Cl_2=2LiCl$	-768.8	3.984	756.0	2518.7
SF_4	$4Li+SF_4=4LiF+S$	-1628.8	4.220	992.1	3331.1
SF_6	$6Li+SF_6=6LiF+S$	-2409.7	4.162	1101.0	3566.1
S_2F_{10}	$10Li+S_2F_{10}=10LiF+2S$	-4016.0	4.162	1054.7	3448.1
SCl_2	$2Li+SCl_2=2LiCl+S$	-740.3	3.836	520.6	1759.8
S_2Cl_2	$2Li+S_2Cl_2=2LiCl+2S$	-729.8	3.782	396.9	1361.3
ClF	$2Li+ClF=LiCl+LiF$	-920.3	4.769	984.4	3741.1
BrF	$2Li+BrF=LiF+LiBr$	-875.8	4.538	542.0	2156.9
BrCl	$2Li+BrCl=LiCl+LiBr$	-780.7	4.046	464.7	1678.0
ClF_3	$4Li+ClF_3=3LiF+LiCl$	-2024.5	5.246	1159.6	4678.1
BrF_3	$4Li+BrF_3=3LiF+LiBr$	-1919.9	4.975	783.1	3238.7
ClF_5	$6Li+ClF_5=5LiF+LiCl$	-3175.9	5.486	1232.8	5126.3
BrF_5	$6Li+BrF_5=5LiF+LiBr$	-2983.9	5.154	919.5	3827.7
IF_5	$6Li+IF_5=LiI(s)+5LiF$	-	-	724.7	2532.0
SOF_2	$4Li+2SOF_2=4LiF+S+SO_2$	-1646.9	4.267	622.8	2288.7
$SOCl_2$	$4Li+2SOCl_2=4LiCl+S+SO_2$	-1441.1	3.734	450.6	1506.6
$SOBr_2$	$4Li+2SOBr_2=4LiBr+S+SO_2$	-	-	257.9	-
SO_2F_2	$2Li+SO_2F_2=2LiF+SO_2$	-1475.5	7.646	525.2	3535.1
SO_2Cl	$2Li+SO_2ClF=LiCl+LiF+S$	-759.2	3.934	452.3	1592.9

F	O_2				
SO_2Cl_2	$2Li+SO_2Cl_2=2LiCl+SO_2$	-748.9	3.881	397.1	1397.6
Na					
X	Chemical Reaction	Δ_rG (kJ mol^{-1})	EMF (V)	Capacity (m A h g^{-1})	Cal. Energy density (W h kg^{-1})
F_2	$2Na+F_2=2NaF$	-1092.6	5.662	1410.7	3614.1
O_2	$4Na+O_2=2Na_2O$	-751.0	1.946	3350.3	1682.9
N_2	$6Na+N_2=2Na_3N$	187.5	-0.32	5740.4	-313.9
S	$2Na+S=Na_2S$	-349.8	1.813	1671.6	1245.0
B	$3Na+B=Na_3B$	-	-	7436.6	-
Si	$4Na+Si=Na_4Si$	-	-	3817.1	-
P	$3Na+P=Na_3P$	-	-	2595.9	-
Cl_2	$2Na+Cl_2=2NaCl$	-768.2	3.981	756.0	1825.6
SF_4	$4Na+SF_4=4NaF+S$	-1463.2	3.791	992.1	2032.0
SF_6	$6Na+SF_6=6NaF+S$	-2161.3	3.733	1101.0	2114.0
S_2F_{10}	$10Na+S_2F_{10}=10NaF+2S$	-3602.0	3.733	1054.7	2067.2
SCl_2	$2Na+SCl_2=2NaCl+S$	-739.7	3.833	520.6	1379.5
S_2Cl_2	$2Na+S_2Cl_2=2NaCl+2S$	-729.2	3.779	396.9	1119.0
ClF	$2Na+ClF=NaCl+NaF$	-878.6	4.553	984.4	2430.1
BrF	$2Na+BrF=NaF+NaBr$	-786.1	4.074	542.0	1507.2
BrCl	$2Na+BrCl=NaCl+NaBr$	-732.1	3.794	464.7	1260.5
ClF_3	$4Na+ClF_3=3NaF+NaCl$	-1900.0	4.923	1159.6	2862.0
BrF_3	$4Na+BrF_3=3NaF+NaBr$	-1747.4	4.528	783.1	2120.9
ClF_5	$6Na+ClF_5=5NaF+NaCl$	-2968.6	5.128	1232.8	3072.5
BrF_5	$6Na+BrF_5=5NaF+NaBr$	-2728.6	4.713	919.5	2422.8
IF_5	$6Na+IF_5=NaI(s)+5NaF$	-	-	724.7	2532.0
SOF_2	$4Na+2SOF_2=4NaF+S+SO_2$	-1481.3	3.838	622.8	1558.1
$SOCl_2$	$4Na+2SOCl_2=4NaCl+S+SO_2$	-1439.9	3.731	450.6	1212.4
$SOBr_2$	$4Na+2SOBr_2=4NaBr+S+SO_2$	-	-	257.9	-
SO_2F_2	$2Na+SO_2F_2=2NaF+SO_2$	-1392.7	7.217	525.2	2613.3
SO_2Cl	$2Na+SO_2ClF=NaCl+Na$	-717.5	3.718	452.3	1211.7

F	$F+SO_2$				
SO_2Cl_2	$2Na+SO_2Cl_2=2NaCl+SO_2$	-748.3	3.878	397.1	1148.8
Mg					
X	chemical reaction	Δ_rG (kJ mol^{-1})	EMF (V)	Capacity (m A h g^{-1})	Cal. Energy density (W h kg^{-1})
F_2	$Mg+F_2=MgF_2$	-1071.1	5.551	1410.7	4775.6
O_2	$2Mg+O_2=2MgO$	-1138.6	2.950	3350.3	3923.6
N_2	$3Mg+N_2=Mg_3N_2$	-400.9	0.693	5740.4	1103.4
S	Mg+S=MgS	-341.8	1.771	1671.6	1684.3
B	$3/2Mg+B=1/2Mg_3B_2$	-	-	7436.6	-
Si	$2Mg+Si=Mg_2Si$	-	-	3817.1	-
P	$3/2Mg+P=1/2Mg_3P_2$	-	-	2595.9	-
Cl_2	$Mg+Cl_2=MgCl_2$	-591.8	3.067	756.0	1726.6
SF_4	$2Mg+SF_4=2MgF_2+S$	-1420.2	3.680	992.1	2518.0
SF_6	$3Mg+SF_6=3MgF_2+S$	-2096.8	3.622	1101.0	2659.9
S_2F_{10}	$5Mg+S_2F_{10}=5MgF_2+2S$	-3494.5	3.622	1054.7	2584.1
SCl_2	$Mg+SCl_2=MgCl_2+S$	-563.3	2.919	520.6	1229.4
S_2Cl_2	$Mg+S_2Cl_2=MgCl_2+2S$	-552.8	2.865	396.9	963.7
ClF	$Mg+ClF=1/2MgCl_2+1/2MgF_2$	-779.7	4.040	984.4	2749.9
BrF	$Mg+BrF=1/2MgF_2+1/2MgBr_2$	-678.3	3.515	542.0	1529.2
BrCl	$Mg+BrCl=1/2MgCl_2+1/2MgBr_2$	-546.8	2.834	464.7	1087.6
ClF_3	$2Mg+ClF_3=3/2MgF_2+1/2MgCl_2$	-1779.6	4.611	1159.6	3504.4
BrF_3	$2Mg+BrF_3=3/2MgF_2+1/2MgBr_2$	-1618.1	4.192	783.1	2422.8
ClF_5	$3Mg+ClF_5=5/2MgF_2+1/2MgCl_2$	-2826.7	4.883	1232.8	3861.0
BrF_5	$3Mg+BrF_5=5/2MgF_2+1/2MgBr_2$	-2577.8	4.453	919.5	2889.5
IF_5	$3Mg+IF_5=1/2MgI_2(s)+5/2MgF_2$		0.000	724.7	2532.0
SOF_2	$2Mg+2SOF_2=2MgF_2+S+$	-1438.3	3.727	622.8	1810.0

	SO_2				
$SOCl_2$	$2Mg+2SOCl_2=2MgCl_2+S+SO_2$	-1087.1	2.817	450.6	1053.8
$SOBr_2$	$2Mg+2SOBr_2=2MgBr_2+S+SO_2$	-	-	257.9	-
SO_2F_2	$Mg+SO_2F_2=MgF_2+SO_2$	-1371.2	7.106	525.2	3014.2
SO_2ClF	$Mg+SO_2ClF=1/2MgCl_2+1/2MgF_2+SO_2$	-618.6	3.206	452.3	1203.1
SO_2Cl_2	$Mg+SO_2Cl_2=MgCl_2+SO_2$	-571.9	2.964	397.1	997.5

Al					
X	Chemical Reaction	Δ_rG (kJ mol^{-1})	EMF (V)	Capacity (m A h g^{-1})	Cal. Energy density (W h kg^{-1})
F_2	$2/3Al+F_2=2/3AlF_3$	-954.1	4.944	1410.7	4733.8
O_2	$4/3Al+O_2=2/3Al_2O_3$	-1054.8	2.733	3350.3	4310.7
N_2	$2Al+N_2=2AlN$	-574.0	0.992	5740.4	1945.0
S	$2/3Al+S=1/3Al_2S_3$	-213.3	1.106	1671.6	1183.9
B	Al+B=AlB	-	-	7436.6	-
Si	$4/3Al+Si=1/3Al_4Si_3$	-	-	3817.1	-
P	Al+P=AlP	-157.9	0.545	2595.9	756.6
Cl_2	$2/3Al+Cl_2=2/3AlCl_3$	-419.2	2.172	756.0	1309.9
SF_4	$4/3Al+SF_4=4/3AlF_3+S$	-1186.1	3.073	992.1	2287.5
SF_6	$2Al+SF_6=2AlF_3+S$	-1745.7	3.015	1101.0	2424.3
S_2F_{10}	$10/3Al+S_2F_{10}=10/3AlF_3+2S$	-2909.3	3.015	1054.7	2348.9
SCl_2	$2/3Al+SCl_2=2/3AlCl_3+S$	-390.7	2.025	520.6	897.2
S_2Cl_2	$2/3Al+S_2Cl_2=2/3AlCl_3+2S$	-380.2	1.970	396.9	690.2
ClF	$2/3Al+ClF=1/3AlCl_3+1/3AlF_3$	-634.9	3.290	984.4	2434.4
BrF	$2/3Al+BrF=1/3AlF_3+1/3AlBr_3$	-530.7	2.750	542.0	1261.1
BrCl	$2/3Al+BrCl=1/3AlCl_3+1/3AlBr_3$	-371.5	1.925	464.7	773.8
ClF_3	$4/3Al+ClF_3=AlF_3+1/3AlCl_3$	-1517.7	3.932	1159.6	3282.8

BrF_3	$4/3Al+BrF_3=AlF_3+1/3AlBr_3$	-1353.4	3.507	783.1	2174.7
ClF_5	$2Al+ClF_5=5/3AlF_3+1/3AlCl_3$	-2447.8	4.228	1232.8	3687.1
BrF_5	$2Al+BrF_5=5/3AlF_3+1/3AlBr_3$	-2196.1	3.794	919.5	2665.5
IF_5	$2Al+IF_5=1/3AlI_3(s)+5/3AlF_3$	-	-	724.7	2532.0
SOF_2	$4/3Al+2SOF_2=4/3AlF_3+S+SO_2$	-1204.3	3.120	622.8	1607.5
$SOCl_2$	$4/3Al+2SOCl_2=4/3AlCl_3+S+SO_2$	-741.9	1.922	450.6	752.4
$SOBr_2$	$4/3Al+2SOBr_2=4/3AlBr_3+S+SO_2$	-	-	257.9	-
SO_2F_2	$2/3Al+SO_2F_2=2/3AlF_3+SO_2$	-1254.2	6.499	525.2	2902.0
SO_2ClF	$2/3Al+SO_2ClF=1/3AlCl_3+1/3AlF_3+SO_2$	-473.8	2.455	452.3	964.1
SO_2Cl_2	$2/3Al+SO_2Cl_2=2/3AlCl_3+SO_2$	-399.3	2.069	397.1	725.2

O_2					
FUEL	Δ_rG (kJ mol^{-1})	n	EMF(V)	Q=ΔH (kJ mol^{-1})	Cal. Energy density (W h kg^{-1})
B	-592.000	3.00	2.045	-636.750	4723.91
Si	-805.000	4.00	2.086	-910.700	3721.63
V	-567.000	3.00	1.959	-609.400	2101.67
Ti	-853.000	4.00	2.210	-944.000	2966.78
TiB_2	-1737.000	10.00	1.800	-1937.500	3227.69
VB_2	-	9.00			
AlB_2	-	9.00			
Li	-280.600	1.00	2.908	-293.950	5216.92
	-578.900	4.00	1.500	-634.300	3504.86
Na	-187.750	1.00	1.946	-207.100	1682.92
Mg	-569.300	2.00	2.950	-601.600	3923.61
Al	-791.150	3.00	2.733	-837.850	4310.74

Zn	-320.500	2.00	1.661	-350.500	1093.85
H_2	-228.600	2.00	1.185	-285.830	3524.78
CO	-257.184	2.00	1.333	-282.964	1623.28
$coal_{(C;\ graphite)}$	-394.364	4.00	1.022	-393.505	2489.13
C_2H_2	-1235.070	10.00	1.280	-1299.571	3235.51
C_2H_4	-1331.430	12.00	1.150	-1411.137	2981.40
$_{(allenic\ )}C_3H_4$	-1859.802	16.00	1.205	-1944.304	3073.99
$_{(propine)}C_3H_4$	-1851.861	16.00	1.200	-1937.610	3060.86
$_{(cyclopropane)}C_3H_6$	-1998.793	18.00	1.151	-2091.225	2983.86
$_{(propylene)}C_3H_6$	-1957.334	18.00	1.127	-2058.423	2921.97
CH_4	-817.889	8.00	1.060	-890.292	2838.47
C_8H_{18}	-5305.899	50.00	1.100	-5512.063	2866.24
C_8H_{18}	-5295.888	50.00	1.098	-5470.558	2860.83
$_{(methanol)}CH3OH$	-702.046	6.00	1.213	-725.965	2436.44
$_{(ethanol)}C_2H_5OH$	-1331.951	12.00	1.150	-1409.694	2604.35
$_{(ethanol)}C_2H_5OH$	-1326.160	12.00	1.145	-1367.519	2593.02
$_{(dimethyl\ ether)}C_2H_6O$	-1387.551	12.00	1.198	-1460.400	2713.06
$C_7H_7NO_2$	-	70.00	-	-3320.945	-
TNT	-	33.00	-	-3353.825	-
N_2H_4	-521.058	12.00	0.450	-556.070	1130.40
$(CH_3)_2NNH_2$	-	24.00	-	-1957.040	-
$(CH_3)_2NNH_3$	-	24.00	-	-1916.840	-
Si_2H_6	-2551.426	14.00	1.889	-2759.504	4068.15
B_2H_6	-1990.987	12.00	1.720	-2165.032	4472.07
$(CH_3CH_2)_3N$	-4119.840	43.00	0.993	-4447.860	2570.66

Typical Battery System						
Battery Type	Δ_rG (kJ mol^{-1})	EMF (V)	Cal. Energy density (W h kg^{-1})	Cal. Energy density (W h L^{-1})	Pra./Cal (max) (%)	※
secondary battery						
Pd-acid	-393.7	2.04	170.2	768.3	29.4	

Na/S	-405.2	2.10	791.7	1178.7	21.5	14
$Na/NiCl_2$	-509.2	2.64	805.6	1231.4	14.3	14
H_2-NiOOH	-132.8	1.38	397.9	1850.7	16.1	
Cd-NiOOH	-248.9	1.29	208.4	778.2	26.4	
Zn-NiOOH	-273.0	1.41	266.2	891.8	31.9	
Fe-NiOOH	-985.3	1.40	281.2	1082.8	19.6	
Fe-O_2	-505.7	1.31	781.6	2796.1	10.2	
	-1015.4	1.32	1218.2	13232.8	6.6	
Fe/AgO	-266.7	1.38	374.4	1738.8	28.0	
$LaNi_5(H_2)$-NiOOH	-125.4	1.30	240.0	-	37.5	14
primary battery						
Li-O_2	-1122.4	2.91	5216.9	5996.6	6.9	17
	-571.0	2.96	3456.8	6100.9	10.5	17
Li/S	-439.0	2.27	2654.0	2901.4	0.0	
Li/I_2	-270.3	2.80	561.0	1938.2	48.1	
Li/MnO_2	-327.8	3.40	969.8	3023.5	23.7	
$Li/(CF)_n$	-299.1	3.10	2189.3	3393.6	26.9	
Li-SO_2	-598.2	3.10	1170.1	6392.0	22.2	
Li-$SOCl_2$	-1441.1	3.73	1506.3	2021.7	22.6	
Li-SO_2Cl_2	-748.9	3.88	1397.3	1938.4	34.4	
Li/CuO	-431.5	2.24	1282.2	3118.6	21.8	
Li/CuS	-385.4	2.00	977.8	2288.5		
Li/FeS	-338.6	1.75	924.1	2122.7		
Li/FeS_2	-721.9	1.87	1358.0	2622.6	19.1	
$Li/AgV_2O_{5.5}$	-1094.1	3.24	943.9	-	28.6	
Li/V_2O_5	-328.0	3.40	482.5	1434.5	12.4	
Li/LiI(Al2O3)/PbI 2,Pb	-367.0	1.90185	214.7	1011.0		
$Li/LiI(Al_2O_3)/PbI_2$, PbS,Pb	-367.0	1.90185	214.7	1011.0		
	-340.3	1.76	373.4	1632.7		
Al-O_2	-3585.4	3.10	3192.0	6727.8	12.5	
Zn-O_2	-320.5	1.66	1093.9	9721.0	33.8	
Zn-Br_2	-355.0	1.84	437.8	aq	17.1	
Zn/HgO	-262.0	1.36	258.1	2527.6	40.7	

Zn/Ag_2O	-309.3	1.60	289.2	2078.0	76.1	
Zn/MnO_2	-271.4	1.41	315.1	1737.7	0.0	
$Zn/KOH/MnO_2$	-308.8	1.60	311.6	1080.4	46.5	14
Cd/HgO	-142.0	0.91	113.7	746.9	48.4	
Cd/AgO	-214.3	1.11	234.1	1168.4		
H_2-O_2	-228.6	1.18	3524.8	g	11.3	
Mg/AgCl	-497.5	2.58	444.4	2108.6	33.8	
Mg/CuCl	-352.0	1.82	439.8	1581.9	18.2	
$Mg/PbCl_2$	-403.6	2.09	370.7	1822.2	21.6	
Mg/Cu_2I_2	-419.1	2.17	287.3	1434.4	27.8	
Mg/CuSCN	-250.9	1.30	260.4	700.6	30.7	
Mg/MnO_2	-511.5	2.65	657.2	2207.0	17.5	

Li-ion battery						
Battery Type	Δ_rG (kJ mol^{-1})	E_{aver} (V)	Capacity (+) (m A h g^{-1})	Cal. Energy density (W h kg^{-1})	Cal. Energy density (W h L^{-1})	*
$Li_2C_6O_6$-Li	-964.9	2.500	589.4	1278.43	-	18
V_2O_5-Li	-781.5	2.700	442.1	1070.98	2327.14	4
$LiCoO_2$-Li	-357.0	3.700	273.8	1013.20	5228.13	1-3
$LiCo_{1/3}Ni_{1/3}Mn_{1/3}O_2$ - Li	-347.3	3.600	277.8	1000.25	4756.17	1,15
MnO_2-Li	-327.8	3.397	308.3	969.79	3023.47	4
$LiMnO_2$-Li	-327.8	3.397	285.5	969.79	4095.42	4
V_2O_5-$Li_{4.4}Si$	-1128.9	2.659	442.1	963.70	2425.72	8
$LiNiO_2$- Li	-337.7	3.500	274.5	960.79	4592.57	1,11
$LiCoO_2$-Si	-1553.4	3.659	273.8	940.65	4517.78	8,11
$LiCo_{1/3}Ni_{1/3}Mn_{1/3}O_2$ - Si	-1510.9	3.559	277.8	927.50	4142.65	8,15
$0.3Li_2MnO_3$-$0.7Li[MnNiCo]_{0.333}O_2$/ Li	-337.7	3.500	261.3	914.46	4066.59	21,22
MnO_2-$Li_{4.4}Si$	-1424.7	3.356	308.3	897.10	3167.55	8
$LiMnO_2$-Si	-1424.7	3.356	285.5	897.10	3602.15	8

$LiNiO_2$- Si	-1468.5	3.459	274.5	891.28	4002.09	8,11
$0.3Li_2MnO_3$-0.7Li[$MnNiCo]_{0.333}O_2$/ Si	-333.7	3.450	261.3	851.00	3593.6	21,22
$LiCoPO_4$-Li	-453.5	4.700	166.6	783.15	2954.83	5,12
$LiCoPO_4$-Si	-1977.9	4.659	166.6	746.70	2752.24	8
$LiCoO_2$-Sn	-1393.0	3.281	273.8	704.35	3878.54	9,11
$LiMnPO_4$-Li	-395.6	4.100	170.9	700.58	2473.74	5
$LiCo_{1/3}Ni_{1/3}Mn_{1/3}O_2$ -Sn	-1350.5	3.181	277.8	690.70	3553.65	9,15
$LiNi_{0.5}Mn_{1.5}O_4$- Li	-449.6	4.660	146.7	683.63	3042.17	6
$LiMnPO_4$-Si	-1723.2	4.059	170.9	666.46	2306.78	8
$LiNiO_2$- Sn	-1308.1	3.081	274.5	662.69	3422.12	9,11
$LiMnO_2$-Sn	-1264.3	2.978	285.5	660.42	3077.44	9
MnO_2-$Li_{4.4}Sn$	-1264.3	2.978	308.3	660.42	2629.58	9
$LiNi_{0.5}Mn_{1.5}O_4$- Si	-1960.9	4.619	146.7	654.75	2826.81	8
V_2O_5-$Li_{4.4}Sn$	-968.4	2.281	442.1	646.65	1950.99	9
$LiCoPO_4$-Sn	-1817.5	4.281	166.6	610.90	2476.27	9
$LiMn_2O_4$- Li	-385.4	3.995	148.2	592.09	2534.14	11
$LiFePO_4$-Li	-332.9	3.450	169.9	586.12	2107.10	5
$LiCoO_2$-C_6	-347.4	3.600	273.8	567.79	1901.04	7,11,16
$LiMn_2O_4$- Si	-1678.4	3.954	148.2	566.04	2355.43	8,11
$LiCo_{1/3}Ni_{1/3}Mn_{1/3}O_2$ - C_6	-337.7	3.500	277.8	556.65	1801.43	7,15
$LiFePO_4$-Si	-1447.3	3.409	169.9	556.64	1959.75	8
$LiNi_{0.5}Mn_{1.5}O_4$- Sn	-1800.5	4.241	146.7	542.13	2539.51	9
$LiNiO_2$- C_6	-328.1	3.400	274.5	537.01	1745.31	7,11
$LiMnPO_4$-Sn	-1562.8	3.681	170.9	536.70	2050.02	9
MnO_2-LiC_6	-318.1	3.297	308.3	532.51	1669.57	7
$LiMnO_2$-C_6	-318.1	3.297	285.5	532.51	1635.84	7
$LiCoPO_4$-C_6	-443.8	4.600	166.6	529.35	1656.71	7
V_2O_5-LiC_6	-752.6	2.600	442.1	499.08	1292.64	7
$LiNi_{0.5}Mn_{1.5}O_4$- C_6	-440.0	4.560	146.7	479.75	1677.84	7
$LiMnPO_4$-C_6	-386.0	4.000	170.9	468.34	1406.78	7
$LiMn_2O_4$- Sn	-1518.0	3.576	148.2	461.19	2085.50	9,11
$LiFePO_4$-Sn	-1286.8	3.031	169.9	439.76	1707.14	9

$LiMn_2O_4$- C_6	-375.8	3.895	148.2	412.78	1409.91	7,11
$LiFePO_4$-C_6	-323.2	3.350	169.9	390.69	1186.57	7
$Li_2C_6H_4O_4$-Li	-162.1	1.400	209.0	277.53	-	19
$LiCoPO_4$-$Li_4Ti_5O_{12}$	-303.9	3.150	166.6	268.97	975.53	10
$Li_2C_8H_4O_4$-Li	-177.5	0.800	346.5	254.36	-	19
$LiNi_{0.5}Mn_{1.5}O_4$-$Li_4Ti_5O_{12}$	-300.1	3.110	146.7	248.28	981.01	10,13
$Li_2C_6O_6$-$Li_6C_6O_6$	-347.3	1.800	294.7	246.44	-	20
$LiCoO_2$-$Li_4Ti_5O_{12}$	-207.4	2.150	273.8	229.66	916.41	10,11
$LiMnPO_4$-$Li_4Ti_5O_{12}$	-246.0	2.550	170.9	220.55	773.71	10
$LiCo_{1/3}Ni_{1/3}Mn_{1/3}O_2$ - $Li_4Ti_5O_{12}$	-197.8	2.050	277.8	220.22	855.84	10,15
$LiNiO_2$- $Li_4Ti_5O_{12}$	-188.1	1.950	274.5	208.50	812.33	10,11
MnO_2-$Li_{7/3}Ti_{5/3}O_4$	-178.5	1.850	308.3	200.81	812.49	10
$LiMnO_2$-$Li_4Ti_5O_{12}$	-178.5	1.850	285.5	200.81	749.65	10
$LiMn_2O_4$- $Li_4Ti_5O_{12}$	-235.4	2.440	148.2	195.89	759.02	10,11
$LiFePO_4$-$Li_4Ti_5O_{12}$	-183.3	1.900	169.9	163.85	580.03	10
V_2O_5- $Li_{7/3}Ti_{5/3}O_4$	-332.9	1.150	442.1	139.72	497.05	

Table S2. Thermodynamic data of typical battery systems. The volumetric energy densities of the batteries containing gas components are not calculated.

Battery Type	Electrochemical Reaction	ΔG (kJ mol^{-1})	EMF (V)	Cal. Energy Density (W h kg^{-1})	Cal. Energy Density (W h L^{-1})
Li/ F_2	$2Li+F_2=2LiF$	-1175	6.090	6294	-
Li/ O_2	$4Li+O_2=2Li_2O$	-1122	2.910	5217	-
Li/ ClF_5(g)	$6Li+ClF_5=5LiF+LiCl$	-3176	5.490	5126	-
Mg/ F_2	$Mg+F_2=MgF_2$	-1071	5.551	4776	-
Al/ F_2	$2/3Al+F_2=2/3AlF_3$	-954.1	4.944	4734	-
B_2H_6(g)/ O_2	$B_2H_6+3O_2=B_2O_3+3H_2O$(l)	-1991	1.720	4472	-
Al/ O_2	$4/3Al+O_2=2/3Al_2O_3$	-1055	2.733	4311	-
Mg/ O_2	$2Mg+O_2=2MgO$	-1139	2.950	3924	-
Na/ F_2	$2Na+F_2=2NaF$	-1093	5.660	3614	-
Li/ SO_2F_2(l)	$2Li+SO_2F_2=2LiF+SO_2$	-1476	7.650	3535	4630
H_2/ O_2	$H_2+1/2O_2=H_2O$	-228.6	1.185	3525	-
C_8H_{18}/ O_2	$C_8H_{18}+25/2O_2=8CO_2+9H_2O$(l)	-5306	1.100	2866	-
CH_4/ O_2	$CH_4+2O_2=CO_2+2H_2O$(l)	-817.9	1.060	2839	-
Li/ S	$2Li+S=Li_2S$	-439.0	2.275	2654	2856
C_2H_5OH(g) / O_2	$C_2H_6O+3O_2=2CO_2+3H_2O$(l)	-1332	1.150	2604	-
Li/ RuF_5	$5Li+RuF_5=5LiF+Ru$	-2157	4.472	2597	5199
Li/ CrO_3	$6Li+CrO_3=3Li_2O+Cr$	-1171	2.023	2297	2828
Li/ $(CF)_n$	$nLi+(CF)_n=nLiF+nC$	-299.1	3.100	2189	3394
Li/ B_2S_3	$6Li+B_2S_3=3Li_2S+2B$	-534.7	1.847	1863	2017
Li/ $Li_2C_6O_6$	$Li_2C_6O_6+4Li=Li_6C_6O_6$	-964.9	2.500	1278	-
C_6/ $LiCoO_2$	$CoO_2+LiC_6=LiCoO_2+C_6$	-347.4	3.600	567.8	1901

Table S3. Thermodynamic data of selected typical lithium battery systems.

Battery type	Electrochemical reaction	ΔG (kJ mol^{-1})	EMF (V)	Energy Density (Wh kg^{-1})	Capacity (+) (mAh g^{-1})
Li/ F_2	$2Li+F_2=2LiF$	-1175	6.090	6294	1411
Li/ O_2	$4Li+O_2=2Li_2O$	-1122	2.910	5217	3350
Li/ ClF_5	$6Li+ClF_5=5LiF+LiCl$	-3176	5.490	5126	1233
Li/ S	$2Li+S=Li_2S$	-439.0	2.275	2654	1672
Li/ RuF_5	$5Li+RuF_5=5LiF+Ru$	-2157	4.472	2597	683.5
Li/ Cl_2	$2Li+Cl_2=2LiCl$	-768.8	3.980	2519	756.0
Li/ CrO_3	$6Li+CrO_3=3Li_2O+Cr$	-1171	2.023	2297	1608
Li/ $(CF)_n$	$nLi+(CF)_n=nLiF+nC$	-299.1	3.100	2189	864.6
Li/ CoF_3	$3Li+CoF_3=3LiF+Co$	-1044	3.607	2121	693.6
Li/ P_2S_5	$5Li+1/2\ P_2S_5=5/2\ Li_2S+P$	-1208	2.131	1958	1206
Li/ P_4O_{10}	$5Li+1/4\ P_4O_{10}=5/2\ Li_2O+P$	-722.2	1.497	1898	1888
Li/ B_2S_3	$3Li+1/2B_2S_3=3/2Li_2S+B$	-534.7	1.847	1863	1365
Li/ CuF_2	$2Li+CuF_2=2LiF+Cu$	-683.4	3.542	1645	527.9
Li/ FeF_3	$3Li+FeF_3=3LiF+Fe$	-791.1	2.733	1644	712.6
Li/ MnO_2	$4Li+MnO_2=2Li_2O+Mn$	-657.3	1.703	1592	1233
Li/ V_2O_5	$5Li+1/2V_2O_5=5/2Li_2O+V$	-693.3	1.437	1533	1474
Li/ $Li_2C_6O_6$	$Li_2C_6O_6+4Li=Li_6C_6O_6$	-964.9	2.500	1278	589.4
Li/ SO_2	$2Li+2SO_2=Li_2S_2O_4$	-598.2	3.100	1170	418.8
Li/ AgO	$2Li+AgO=Li_2O+Ag$	-575.0	2.980	1160	432.7
Li/ MnO_2	$Li+MnO_2=LiMnO_2$	-327.8	3.400	969.8	308.1
C_6/ $LiCoO_2$	$CoO_2+LiC_6= LiCoO_2+C_6$	-347.4	3.600	567.8	237.8

Table S4. Thermodynamic data of all lithium battery systems calculated.

Metallic lithium battery					
Battery Type	Electrochemical Reaction	ΔG_r (kJ mol^{-1})	EMF (V)	Energy Density (Wh kg^{-1})	Capacity (+) (mAh g^{-1})
Li/ F_2	$2Li+F_2=2LiF$	-1175.4	6.090	6293.5	1410.7
Li/ O_2	$4Li+O_2=2Li_2O$	-1122.4	2.910	5216.9	3350.3
Li/ ClF_5	$6Li+ClF_5=5LiF+LiCl$	-3175.9	5.490	5126.3	1232.8
Li/ClF_3	$4Li+ClF_3=3LiF+LiCl$	-2024.5	5.250	4678.1	1159.6
Li/ SO_2F_2	$2Li+SO_2F_2=2LiF+SO_2$	-1475.5	7.650	3535.1	525.2
Li/BrF_5	$6Li+BrF_5=5LiF+LiBr$	-2983.9	5.150	3827.7	919.5
Li/(g)ClF	$2Li+ClF=LiCl+LiF$	-920.3	4.770	3741.2	984.4
Li/(g)SF_6	$6Li+SF_6=6LiF+S$	-2409.7	4.160	3566.1	1101.0
Li/ S_2F_{10}	$10Li+S_2F_{10}=10LiF+2S$	-4016.0	4.160	3448.1	1054.7
Li/ (g)SF_4	$4Li+SF_4=4LiF+S$	-1628.8	4.220	3331.1	992.1
Li/ BrF_3	$4Li+BrF_3=3LiF+LiBr$	-1919.9	4.970	3238.7	783.1
Li/ S	$2Li+S=Li_2S$	-439.0	2.270	2654.0	1671.6
Li/ RuF_5	$5Li+RuF_5=5LiF+Ru$	-2157.2	4.472	2596.7	683.5
Li/ Cl_2	$2Li+Cl_2=2LiCl$	-768.8	3.980	2518.7	756.0
Li/ CrO_3	$6Li+CrO_3=3Li_2O+Cr$	-1171.0	2.023	2296.6	1608.2
Li/ SOF_2	$4Li+2SOF_2=4LiF+S+SO_2$	-1646.9	4.270	2288.7	622.8
Li/ $(CF)_n$	$nLi+(CF)_n=nLiF+nC$	-299.1	3.100	2189.3	864.6
Li/ BrF	$2Li+BrF=LiF+LiBr$	-875.8	4.540	2156.9	542.0
Li/ CoF_3	$3Li+CoF_3=3LiF+Co$	-1044.1	3.607	2120.8	693.6
Li/ P_2S_5	$5Li+1/2P_2S_5=5/2\ Li_2S+P$	-1207.9	2.131	1957.7	1205.8
Li/ SeO_2	$4Li+SeO_2=2Li_2O+Se$	-950.9	2.464	1904.1	966.2
Li/ P_4O_{10}	$5Li+1/4P_4O_{10}=5/2\ Li_2O+P$	-722.2	1.497	1898.3	1888.2
Li/ As_2O_5	$5Li+1/2As_2O_5=5/2Li_2O+As$	-1011.9	2.097	1878.5	1166.1
Li/ B_2S_3	$3Li+1/2B_2S_3=3/2Li_2S+B$	-534.7	1.847	1862.8	1364.8
Li/ SCl_2	$2Li+SCl_2=2LiCl+S$	-740.3	3.840	1759.8	520.6

Li/ BrCl	2Li+BrCl=LiCl+LiBr	-780.7	4.050	1678.0	464.7
Li/ CuF_2	2Li+CuF_2=2LiF+Cu	-683.4	3.542	1644.7	527.9
Li/ FeF_3	3Li+FeF_3=3LiF+Fe	-791.1	2.733	1644.1	712.6
Li/ Ag_2O_3	3Li+1/2Ag_2O_3=3/2Li_2O+Ag	-902.5	3.118	1641.9	609.7
Li/ MnF_3	3Li+MnF_3=3LiF+Mn	-763.1	2.636	1596.7	718.3
Li/ SO_2ClF(g)	2Li+SO_2ClF=LiCl+LiF+SO_2	-759.2	3.930	1592.9	452.3
Li/ MnO_2	4Li+MnO_2=2Li_2O+Mn	-657.3	1.703	1591.8	1233.1
Li/ NbF_5	5Li+NbF_5=5LiF+Nb	-1239.5	2.569	1546.7	713.2
Li/ SiS_2	4Li+SiS_2=2Li_2S+Si	-665.4	1.724	1540.5	1162.5
Li/ V_2O_5	5Li+1/2V_2O_5=5/2Li_2O+V	-693.3	1.437	1532.6	1473.6
Li/ MoO_3	6Li+MoO_3=3Li_2O+Mo	-1015.6	1.754	1520.1	1117.2
Li/ $MoCl_6$	6Li+$MoCl_6$=6LiCl+Mo	-1915.4	3.309	1518.8	521.0
Li/ $SOCl_2$	4Li+2$SOCl_2$=4LiCl+S+SO_2	-1441.1	3.730	1506.6	450.6
Li/ RuO_2	4Li+RuO_2=2Li_2O+Ru	-842.4	2.183	1454.9	805.6
Li/ TiF_4	4Li+TiF_4=4LiF+Ti	-791.8	2.052	1450.6	865.5
Li/ CrO_2	4Li+CrO_2=2Li_2O+Cr	-577.5	1.496	1435.4	1276.3
Li/ NiF_2	2Li+NiF_2=2LiF+Ni	-571.3	2.961	1435.2	554.4
Li/ CrF_3	3Li+CrF_3=3LiF+Cr	-659.7	2.279	1411.5	737.7
Li/ SO_2Cl_2	2Li+SO_2Cl_2=2LiCl+SO_2	-748.9	3.880	1397.6	397.2
Li/ NiS_2	4Li+NiS_2=2Li_2S+Ni	-753.3	1.952	1389.5	872.8
Li/ Co_3O_4	8/3Li+1/3Co_3O_4=4/3Li_2O+Co	-490.3	1.906	1378.7	890.4
Li/ FeS_2 (marcasite)	4Li+FeS_2=2Li_2S+Fe	-721.9	1.870	1358.0	893.4
Li/ $MoCl_5$	5Li+$MoCl_5$=5LiCl+Mo	-1499.0	3.107	1352.3	490.5
Li/ CoS_2	4Li+CoS_2=2Li_2S+Co	-732.4	1.898	1348.7	871.1
Li/ $FeS_{2(pyrite)}$	4Li+FeS_2=2Li_2S+Fe	-711.1	1.843	1337.0	893.6
Li/ CoF_2	2Li+CoF_2=2LiF+Co	-528.2	2.737	1324.1	533.0
Li/ Cr_2S_3	3Li+1/2Cr_2S_3=3/2 Li_2S+Cr	-574.6	1.985	1319.9	803.3
Li/ FeF_2	2Li+FeF_2=2LiF+Fe	-506.8	2.626	1306.8	571.2
Li/ Fe_2O_3	3Li+1/2Fe_2O_3=3/2 Li_2O+Fe	-470.7	1.626	1298.8	1007.0
Li/ As_4O_6	6Li+1/2	-533.7	1.913	1284.4	812.8

	As_2O_6=3Li_2O+As				
Li/ CuO	2Li+CuO=Li_2O+Cu	-431.5	2.236	1282.9	673.9
Li/ $Li_2C_6O_6$	$Li_2C_6O_6$+4Li=$Li_6C_6O_6$	-964.9	2.500	1278.4	589.4
Li/ GaF_3	3Li+GaF_3=3LiF+Ga	-677.8	2.342	1276.1	634.5
Li/ GeO_2	4Li+GeO_2=2Li_2O+Ge	-601.0	1.557	1260.9	1024.5
Li/ Cu_2O	Li+1/2Cu_2O=1/2Li_2O+ Cu	-354.5	3.675	1254.8	374.6
Li/ $FeCl_3$	3Li+$FeCl_3$=3LiCl+Fe	-819.2	2.830	1243.3	495.7
Li/ MnS_2	4Li+MnS_2=2Li_2S+Mn	-653.0	1.692	1235.4	900.4
Li/ P_4S_3	3/2Li+1/4P_4S_3=3/4Li_2S +P	-289.5	2.000	1229.0	730.6
Li/ B_2O_3	3Li+1/2B_2O_3=3/2Li_2O+ B	-244.7	0.845	1221.5	2309.7
Li/ GeS_2	4Li+GeS_2=2Li_2S+Ge	-723.4	1.874	1221.3	783.8
Li/ $RuCl_3$	3Li+$RuCl_3$=3LiCl+Ru	-993.5	3.432	1209.0	387.6
Li/ Fe_3O_4	8/3Li+1/3Fe_3O_4=4/3Li_2 O+Fe	-409.8	1.593	1189.6	926.1
Li/ $MoCl_4$	4Li+$MoCl_4$=4LiCl+Mo	-1135.6	2.942	1188.0	450.9
Li/ WCl_6	6Li+WCl_6=6LiCl+W	-1850.4	3.196	1173.0	405.5
Li/ SO_2	2Li+2SO_2=$Li_2S_2O_4$	-598.2	3.100	1170.1	418.8
Li/ AgO	2Li+AgO=Li_2O+Ag	-575.0	2.980	1159.6	432.7
Li/ VF_3	3Li+VF_3=3LiF+V	-536.4	1.853	1157.3	744.9
Li/ Ni_3S_4	8/3Li+1/3Ni_3S_4=4/3Li_2S +Ni	-488.0	1.897	1130.1	704.5
Li/ $NbCl_5$	5Li+$NbCl_5$=5LiCl+Nb	-1238.8	2.568	1128.7	496.0
Li/ Mn_2O_3	3Li+1/2Mn_2O_3=3/2Li_2O +Mn	-401.3	1.386	1117.3	1018.6
Li/ $CuCl_2$	2Li+$CuCl_2$=2LiCl+Cu	-593.1	3.074	1110.7	398.7
Li/ As_2S_3	3Li+1/2As_2S_3=3/2 Li_2S+As	-574.2	1.984	1108.8	653.6
Li/ NiO	2Li+NiO=Li_2O+Ni	-349.5	1.811	1096.1	717.6
Li/ ZnF_2	2Li+ZnF_2=2LiF+Zn	-462.1	2.395	1094.6	518.5
Li/ CoO	2Li+CoO=Li_2O+Co	-347.0	1.798	1085.3	715.4
Li/ Ni CO_3	2Li+$NiCO_3$=Li_2CO_3+Ni	-514.2	2.665	1077.4	451.6
Li/ $Fe_2(SO_4)_3$	3Li+1/2 $Fe_2(SO_4)_3$=3/2Li_2SO_4+ Fe	-851.2	2.941	1071.0	402.1
Li/ WCl_5	5Li+WCl_5+5LiCl+W	-1520.0	3.151	1066.7	371.1
Li/ $CuSO_4$	2Li+$CuSO_4$=Li_2SO_4+C	-659.5	3.418	1055.9	335.8

	u				
Li/ MoO_2	$4Li+MoO_2=2Li_2O+Mo$	-589.4	1.527	1051.5	837.9
Li/ BeS	$2Li+BeS=Li_2S+Be$	-206.0	1.068	1041.2	1304.9
Li/ Co CO_3	$2Li+CoCO_3=Li_2CO_3+Co$	-495.3	2.567	1035.9	450.7
Li/ $CrCl_3$	$3Li+CrCl_3=3LiCl+Cr$	-667.1	2.305	1034.2	507.8
Li/ N_2	$6Li+N_2=2Li_3N$	-257.2	0.440	1025.6	5740.4
Li/ CuF	Li+CuF=LiF+Cu	-327.7	3.396	1017.2	324.7
Li/ FeO	$2Li+FeO=Li_2O+Fe$	-309.8	1.605	1003.8	746.1
Li/ VCl_3	$3Li+VCl_3=3LiCl+V$	-641.9	2.218	1001.0	511.2
Li/ $NiCl_2$	$2Li+NiCl_2=2LiCl+Ni$	-509.8	2.6	987.0	413.6
Li/ $NbCl_4$	$4Li+NbCl_4=4LiCl+Nb$	-932.1	2.4	986.4	456.7
Li/ $GaCl_3$	$3Li+GaCl_3=3LiCl+Ga$	-698.4	2.4	985.2	456.6
Li/ Al_2S_3	$3Li+1/2Al_2S_3=3/2Li_2S+Al$	-338.5	1.2	980.4	1070.9
Li/ CuS	$2Li+CuS=Li_2S+Cu$	-385.4	2.0	977.7	560.6
Li/ Co_3S_4	$8/3Li+1/3Co_3S_4=4/3Li_2S+Co$	-423.0	1.6	977.6	702.8
Li/ $FeCO_3$	$2Li+FeCO_3=Li_2CO_3+Fe$	-465.4	2.4	973.3	450.7
Li/ MnO_2	$Li+MnO_2=LiMnO2$	-327.8	3.4	969.8	308.1

Table S5. Thermodynamic data of lithium-ion battery systems with high gravimetric energy densities.

Battery Type	ΔG (kJ mol^{-1})	E_{aver} (V)	Capacity (+) (mAh g^{-1})	Capacity (-) (mAh g^{-1})	Cal. Energy Density (Wh kg^{-1})	Cal. Energy Density (Wh L^{-1})
V_2O_5-$Li_{4.4}Si$	-1128.9	2.660	442.1	2011.5	963.7	2425.7
$LiCoO_2$-Si	-1553.4	3.660	273.8	4198.8	940.7	4517.8
$Li(CoNiMn)_{1/3}O_2$-Si	-1510.9	3.560	277.8	4198.8	927.5	4142.7
MnO_2-$Li_{4.4}Si$	-1424.7	3.360	308.3	2011.5	897.1	3167.6
$0.3Li_2MnO_3$-$0.7Li[MnNiCo]_{0.333}O_2$-Si	-333.75	3.450	261.3	4198.8	851.0	3593.6
$LiCoPO_4$-Si	-1977.9	4.660	166.6	4198.8	746.7	2752.2
$LiCoO_2$-Sn	-1393.0	3.280	273.8	993.40	704.4	3878.5
$Li(CoNiMn)_{1/3}O_2$-Sn	-1350.5	3.180	277.8	993.40	690.7	3553.7
$LiMnPO_4$-Si	-1723.2	4.060	170.9	4198.8	666.5	2306.8
$LiMnO_2$-Sn	-1264.3	2.980	285.5	993.4	660.4	3077.4

Table S6. Capacity values of typical lithium-free cathodes.

Formula	Theoretical Capacity (mAh g^{-1})	Practical Capacity (mAh g^{-1})	Charge Transfer (max)	Voltage (V) (vs.Li+/Li)
CrO_3	1608	-	6.0	2.023
P_2S_5	1206	-	10.0	2.131
SeO_2	966.2	-	4.0	2.464
TiF_4	865.5	-	4.0	2.052
$(CF)_n$	864.3	220.0	1.0	3.100
$Li_{1.2}V_3O_8$	816.0	250.0	8.8	2.500*
RuO_2	805.6	-	4.0	2.183
CrF_3	737.7	-	3.0	2.279
MnF_3	718.3	-	3.0	2.636
FeF_3	712.6	-	3.0	2.733
CoF_3	693.6	-	3.0	3.607
RuF_5	683.5	-	5.0	4.472
CuO	673.9	187.0	2.0	2.236
Cr_8O_{21}	642.0	265.0	18.0	3.000*
$Li_2C_6O_6$	589.0	300.0	4.0	2.500*
NiF_2	554.4	-	2.0	2.961
CuF_2	527.9	-	2.0	3.542
VCl_3	511.2	-	3.0	2.218
$Cu_{2.33}V_4O_{11}$	475.0	270.0	9.3	2.700*
$NiCO_3$	451.6	-	2.0	2.665
V_2O_5	442.1	400.0	3.0	2.700
MnO_2	308.3	150.0	1.0	3.400

Table S7. Capacity values of lithium-contained cathodes.

Formula	Theoretical Capacity (mAh g^{-1})	Practical Capacity (mAh g^{-1})	Charge Transfer (max)	Voltage (V) (vs.Li+/Li)
$0.3Li_2MnO_3$-$0.7Li[Mn_{0.333}Ni_{0.333}Co_{0.333}]O_2$	261.3	250.0	1.0	3.500*
$LiMnO_2$	285.5	190.0	1.0	3.400*
$LiCo_{1/3}Ni_{1/3}Mn_{1/3}O_2$	277.8	118.0	1.0	3.60
$LiNiO_2$	274.5	170.0	1.0	3.50
$LiCoO_2$	273.8	140.0	1.0	3.70
$LiMnPO_4$	170.9	168.0	1.0	4.100
$LiFePO_4$	169.9	160.0	1.0	3.450
$LiCoPO_4$	166.7	100.0	1.0	4.700
$LiMn_2O_4$	148.2	110.0	1.0	3.990
$LiNi_{0.5}Mn_{1.5}O_4$	146.7	110.0	1.0	4.660
$LiCo_{0.5}Mn_{1.5}O_4$	146.6	130.0	1.0	5.100
$LiCoMnO_4$	145.0	130.0	1.0	5.100
Li_3CrO_3	665.5	-	3.0	-
$Li_3CrO_2F_2$	563.0	-	3.0	-
Li_2NiO_2	512.6	200.0	2.0	-
Li_3CrF_6	430.4	-	3.0	-
Li_2MnBO_3F	365.6	-	2.0	-
Li_2NiF_4	360.8	-	2.0	-
Li_2MnSiO_4	333.1	150.0	2.0	3.000*
$Li_3Cr(PO_4)_2$	305.0	-	3.0	-
Li_2CrPO_4O	302.0	-	2.0	-
Li_2CrMnO_4	290.0	-	2.0	-
$LiNi_{0.5}Ti_{1.5}O_4$	155.7	-	1.0	-
$LiCrMnO_4$	150.7	75.0	1.0	4.800
$LiCr_{0.5}Mn_{1.5}O_4$	149.4	125.0	1.0	4.800
$LiNiVO_4$	148.4	40.0	1.0	4.800
$LiFe_{0.5}Mn_{1.5}O_4$	147.9	125.0	1.0	4.900
$Li_{1.01}Cu_{0.32}Mn_{1.67}O_4$	147.8	71.0	1.0	4.900

Table S8. Capacity values of typical anodes.

Formula	Capacity (mA h g^{-1})	Charge Transfer (max)	Voltage (V) (vs.Li+/Li)
Si	4200	4.4	0.04000
BN	3240	3.0	-0.3448
AlN	1962	3.0	-0.5472
P_4O_{10}	1888	20.0	1.497
SiO_2	1784	4.0	0.6895
Al_2O_3	1577	6.0	0.1750
V_2O_5	1474	10.0	1.437
B_2S_3	1365	6.0	1.847
TiO_2-R	1342	1.0	0.6046
TiN	1299	3.0	-0.3980
VO_2	1293	4.0	-0.5080
CrO_2	1276	4.0	1.496
MnO_2	1233	4.0	1.703
Sn	993.4	4.4	0.5040
TiO	839.3	2.0	0.3431
VO	800.8	2.0	0.8136
$Al_2(SO_4)_3$	470.0	6.0	0.7913
$LiTiS_2$	225.4	1.0	0.5000*
$LiVS_2$	219.7	1.0	1.000*
$Li_4Ti_5O_{12}$	175.1	3.0	1.550*

Table S9. Capacity values calculated in all.

Capacity					
Chemical formula	Capacity (m A h g^{-1})	Chemical formula	Capacity (m A h g^{-1})	Chemical formula	Capacity (m A h g^{-1})
LiF	1033.23	Li_2S	1166.6	$LiBO_2$	538.7
BeF_2	1140.27	BeS	1304.90	$NaBO_2$	407.31
NaF	638.31	B_2S_3	1364.84	$Mg(BO_2)_2$	487.62
MgF_2	860.37	Na_2S	686.81	$Al\ (BO_2)_3$	517.35
AlF_3	957.46	MgS	950.89	KBO_2	327.21
KF	461.32	Al_2S_3	1070.91	$Sc(BO_2)_3$	463.72
CaF_2	686.56	SiS_2	1162.53	$Ti\ (BO_2)_4$	489.28
ScF_3	788.65	P_4S_3	730.64	$V(BO_2)_5$	505.70
TiF_3	766.76	P_4S_7	1077.11	$Cr(BO_2)_6$	520.65
TiF_4	865.53	P_2S_5	1205.76	$Mn\ (BO_2)_3$	438.48
VF_3	744.92	K_2S	486.14	$Fe\ (BO_2)_2$	378.91
CrF_3	737.71	CaS	743.00	$Co\ (BO_2)_3$	429.13
MnF_2	576.78	Sc_2S_3	864.05	$Ni(BO_2)_3$	429.68
MnF_3	718.32	TiS_2	957.20	$Cu(BO_2)_2$	359.35
FeF_2	571.20	TiS	670.60	$Zn(BO_2)_2$	354.96
FeF_3	712.55	Ti_2S_3	837.84	$Ga(BO_2)_3$	405.76
CoF_2	553.00	VS	645.76	$Ge(BO_2)_4$	439.58
CoF_3	693.57	V_2S_3	811.83	$Y\ (BO_2)_3$	369.95
NiF_2	554.38	VS_2	931.63	$Zr\ (BO_2)_4$	408.45
CuF	324.69	V_2S_5	1022.12	$Nb\ BO_2$	197.48
CuF_2	527.88	CrS	637.66	$MoBO_2$	193.16
ZnF_2	518.47	Cr_2S_3	803.28	$Ru(BO_2)_2$	287.12
GaF_3	634.51	MnS	616.10	$Ag\ BO_2$	177.87
RbF	256.56	MnS_2	900.36	$La\ (BO_2)_3$	300.76
YF_3	551.09	FeS	609.74	$Ce(BO_2)_4$	344.31
ZrF_2	414.82	$FeS_{2(marcasite)}$	893.55	$W\ (BO_2)_6$	364.89

ZrF_3	542.47	$FeS_{2(pyrite)}$	893.55	$Be_3(BO_3)_2$	1111.65
ZrF_4	641.11	CoS	589.05	$Ca_3(BO_3)_2$	676.08
NbF_5	713.19	Co_2S_3	751.21	$Li_2\ CO_3$	725.43
RuF_3	508.68	CoS_2	871.13	$Be\ CO_3$	776.61
RuF_5	683.49	Co_3S_4	702.84	$B_2(CO_3)_3$	797.46
AgF	211.26	NiS	590.60	$Na_2\ CO_3$	505.74
SnF_2	342.06	Ni_3S_4	704.50	$Mg\ CO_3$	653.75
LaF_3	410.43	Ni_3S_2	446.30	$Al_2(\ CO_3)_3$	687.24
CeF_3	407.91	NiS_2	872.83	$K_2\ CO_3$	387.85
Li_2O	1793.85	CuS	560.63	$CaCO_3$	535.56
BeO	2143.12	Cu_2S	336.79	$Sc\ _2(CO_{3)3}$	595.72
B_2O_3	2309.73	ZnS	550.02	$Ti\ (CO_3)_2$	638.57
Na_2O	864.85	Ga_2S_3	682.42	$V_2(CO_3)_5$	666.82
MgO	1329.95	GaS	526.61	$Cr\ (CO_3)_3$	693.07
Al_2O_3	1577.15	GeS	511.94	$MnCO_3$	466.33
SiO_2 quartz	1784.25	GeS_2	783.83	$Fe_2(CO_3)_3$	551.25
SiO_2 high cristobalite	1784.25	As_2S_3	653.58	$FeCO_3$	450.66
P_4O_{10}	1888.16	Se_2S_6	918.08	$Co\ CO_3$	450.66
K_2O	569.06	Se_4S_4	482.79	$Ni\ CO_3$	451.57
CaO	955.87	RuS_2	648.94	$CuCO_3$	433.84
Sc_2O_3	1166.04	Y_2S_3	586.87	$Zn\ CO_3$	427.46
TiO	839.30	ZrS_2	690.06	$Ga_2(CO_3)_3$	503.36
Ti_2O_3	1118.81	NbS_2	690.06	$Ge(CO_3)_2$	556.46
Ti_3O_5	1198.64	MoS_2	669.73	$Y_2(CO_3)_3$	449.39
TiO_2-R	1342.32	Mo_2S_3	558.21	$ZrCO_3$	354.44
TiO2-B	1342.32	$Ag_2S_{(argentite)}$	216.31	$Nb_2\ CO_3$	218.06
TiO_2-A	1342.32	LaS	313.52	Mo_2CO_3	212.80
VO	800.75	La_2S_3	429.96	Ru_2CO_3	204.47
V_2O_3	1072.91	CeS	311.31	$Ag_2\ CO_3$	194.39
VO_2	1292.56	WS_2	432.33	$La\ _2(CO_3)_3$	351.23
V_3O_5	1151.16	Na_2S_2	486.80	$Ce_2(CO_3)_3$	349.39
V_2O_5	1473.58	Li_3N	2308.49	$W\ (CO_3)_3$	441.94

CrO_2	1276.33	Be_3N_2	2921.14	Li_3PO_4	694.37
Cr_2O_3	1058.01	BN	3239.66	$Be_{3(}PO_{4)2}$	741.12
Cr_3O_4	947.66	(CN)	3090.39	Na_3PO_4	490.45
CrO_3	1608.17	Na_3N	969.00	$Mg_3(PO_4)_2$	611.77
MnO_2	1233.14	Mg_3N2	1593.29	Al PO_4	659.31
Mn_2O_3	1018.58	AlN	1961.64	K_3 PO_4	378.79
MnO	755.63	Si_3N_4	2292.62	$Ca_3(PO_4)_2$	518.44
Mn_3O_4	937.06	K_3N	612.36	Sc PO_4	574.61
FeO	746.10	Ca_3N_2	1084.73	Ti $_3(PO_4)_4$	614.37
Fe_2O_3	1007.01	ScN	1363.65	V_3 $(PO_4)_5$	640.49
Fe_3O_4	926.05	TiN	1299.49	$CrPO_4$	547.09
CoO	715.35	VN	1237.97	Mn PO_4	536.35
Co_3O_4	890.42	CrN	1218.19	Mn3(PO_4)2	453.29
NiO	717.64	Cr_2N	681.40	Fe PO_4	533.13
Ni_2O_3	972.33	Mn_4N	343.96	$Co3(PO_4)_2$	438.48
CuO	673.86	Mn_5N_2	531.24	$Ni_3(PO_4)_2$	439.34
Cu_2O	374.61	Fe_2N	639.67	$Cu_3(PO_4)_2$	422.53
ZnO	658.60	Fe_4N	338.71	$Zn_3(PO_4)_2$	416.48
Ga_2O_3	857.90	Co_3N	421.39	Ga PO_4	488.20
GeO	604.73	NiN	1105.97	$Ge_3(PO_4)_4$	538.00
GeO_2	1024.53	Cu_3N	392.90	Y PO_4	437.27
As_4O_6	812.81	Zn_3N_2	717.31	Zr $_3(PO_4)_2$	346.27
As_2O_5	1166.09	GaN	960.28	Nb_3 PO_4	215.16
SeO_2	966.17	Ge_3N_4	1174.01	Mo_3PO_4	210.05
Y_2O_3	712.14	As_3N_5	1363.71	Ru_3 PO_4	201.93
ZrO_2	870.01	SeN_2	1503.26	Ag_3 PO_4	192.09
NbO	492.19	YN	781.29	La PO_4	343.79
NbO_2	858.30	ZrN	764.08	$CePO_4$	342.02
Nb_2O_5	1008.29	NbN	752.05	W $(PO_4)_2$	430.22
MoO_2	837.94	MoN	731.30	Li_2 SO_4	487.54
MoO_3	1117.20	RuN	698.70	Be SO_4	510.13
RuO_2	805.64	Ag_3N	238.16	Na_2 SO_4	377.37
RuO_4	1298.93	LaN	525.82	Mg SO_4	445.32
AgO	432.74	CeN	521.69	$Al_2($ $SO_4)_3$	469.99

Ag_2O	231.31	WN_2	759.05	$AlK(SO_4)_2$	415.19
Ag_2O_3	609.74	NaN_3	179.81	$K_2\ SO_4$	307.60
La_2O_3	493.57	KN_3	162.28	$CaSO_4$	393.73
CeO_2	622.87	LiCl	632.20	$Sc\ _2(SO_{4)3}$	425.30
Ce_2O_3	489.93	$BeCl_2$	670.72	$Ti\ (SO_4)_2$	446.70
WO_2	496.69	PCl_5	643.53	$V_2(SO_4)_5$	460.35
WO_3	693.62	NaCl	458.59	$Cr\ 2(SO_4)_3$	410.03
Na_2O_2	687.41	$MgCl_2$	562.99	$MnSO_4$	354.98
K_2O_2	486.43	$AlCl_3$	603.00	$FeSO_4$	352.86
Ag_2O_2	216.37	KCl	359.50	$Fe_2(SO_4)_3$	402.14
Li_2O_2	1168.31	$CaCl_2$	482.98	$Co\ SO_4$	345.83
NaO_2	487.40	$ScCl_3$	531.37	$Ni\ SO_4$	346.37
KO_2	376.97	$TiCl_2$	451.30	$CuSO_4$	335.84
CaO_2	371.84	$TiCl_3$	521.34	$Zn\ SO_4$	332.00
Li_3P	1552.30	VCl_2	439.92	$Y_2(SO_4)_3$	345.08
Be_3P_2	1807.16	VCl_3	511.15	$Zr(SO_{4)2}$	378.35
BP	1924.20	$CrCl_2$	436.14	Nb_2SO_4	190.16
Na_3P	804.50	$CrCl_3$	507.75	Mo_2SO_4	186.16
Mg_3P_2	1192.38	$MnCl_2$	425.95	Ru_2SO_4	179.75
AlP	1387.35	$FeCl_2$	422.90	$Ag_2\ SO_4$	171.91
Si_3P_4	1545.11	$FeCl_3$	495.70	$La\ _2(SO_4)_3$	284.11
K_3P	542.29	$CoCl_2$	412.84	$Ce_2(SO_4)_3$	282.90
Ca_3P_2	882.68	$NiCl_2$	413.60	$W\ (SO_4)_3$	340.67
ScP	1058.93	CuCl	270.72	F_2	1410.72
TiP	1019.83	$CuCl_2$	398.68	O_2	3350.30
(VP)	981.55	$ZnCl_2$	393.68	N_2	5740.41
CrP	969.08	$GaCl_3$	456.63	S	1671.64
MnP	935.89	$AsCl_5$	531.38	B	7436.57
Mn_2P	570.85	$SeCl_4$	485.59	Si	3817.11
FeP	926.12	YCl_3	411.77	P	2595.88
Fe_2P	563.59	$ZrCl_2$	330.62	Cl_2	755.97
Fe_3P	405.04	$ZrCl_3$	406.94	$(g)SF_4$	992.10
Co_2P	540.20	$ZrCl_4$	460.04	$(g)SF_6$	1101.00
Ni_2P	541.95	$NbCl_5$	496.01	S_2F_{10}	1054.69

Ni_3P	388.32	$NbCl_4$	456.74	SCl_2	520.56
Ni_5P_2	452.45	$MoCl_4$	450.91	S_2Cl_2	396.95
CuP_2	1281.41	$MoCl_5$	490.50	(g)ClF	984.41
Cu3P	362.82	$MoCl_6$	520.99	BrF	541.98
Zn_3P_2	623.00	$RuCl_3$	387.62	BrCl	464.67
GaP	798.48	AgCl	187.00	ClF_3	1159.63
GeP	776.00	$SnCl_2$	282.69	BrF_3	783.10
Ge_3P_4	940.91	$LaCl_3$	327.83	(g)ClF_5	1232.77
As_3P_5	1058.97	$CeCl_3$	326.22	BrF_5	919.45
$Se(P)_2$	1141.23	WCl_2	210.42	IF_5	724.70
YP	670.71	WCl_4	329.20	SOF_2	622.84
ZrP_2	1049.86	WCl_5	371.10	(g)$SOCl_2$	450.55
NbP	649.05	WCl_6	405.51	$SOBr_2$	257.86
MoP	633.53	$0.3Li_2MnO_3$-0.7Li$[MnNiCo]_{1/3}O_2$	262.00	SO_2F_2	645.33
RuP	608.92	$MnO_{2(intercalation)}$	308.30	(g)SO_2ClF	452.28
AgP2	946.96	$V_2O_{5(intercalation)}$	442.10	SO_2Cl_2	397.15
AgP3	1201.32	$Li_2C_6O_6$	589.40	$LiCoO_2$	273.80
LaP	473.30	$Li_6C_6O_6$	294.70	$LiNiO_2$	274.50
Ce_3P_4	590.94	$Li_2C_6H_4O_4$	209.00	$LiMnO_2$	285.50
WP_2	654.26	$Li_2C_8H_4O_4$	346.50	$LiMn_2O_4$	148.20
-	-	C_6	371.90	$LiFePO_4$	169.90
-	-	Si	4198.80	$LiCoPO_4$	166.60
-	-	Sn	993.40	$LiMnPO_4$	170.90
-	-	$Li_4Ti_5O_{12}$	175.10	$LiNi_{0.5}Mn_{1.5}O_4$	146.70
-	-			$LiCo_{1/3}Ni_{1/3}Mn_{1/3}O_2$	277.80

Table S10. Calculated EMF values (V) of conversion reactions between binary transition mental compounds and lithium.

$bLi + 1/a\ M_aX_b = b/aLi_aX + M$				
M_aX_b	ΔG (kJ mol^{-1})	EMF (V)	Capacity (+) (mAh g^{-1})	Energy Density (Wh kg^{-1})
TiF_3	-401.1	1.386	766.8	886.5
TiF_4	-791.8	2.052	865.5	1451
VF_3	-536.4	1.853	744.9	1157
CrF_3	-659.7	2.279	737.7	1412
MnF_2	-368.3	1.909	576.8	957.8
MnF_3	-763.1	2.636	718.3	1597
FeF_2	-506.8	2.626	571.2	1307
FeF_3	-791.0	2.733	712.6	1644
CoF_2	-528.2	2.737	553.0	1324
CoF_3	-1044	3.607	693.6	2121
NiF_2	-571.3	2.961	554.4	1435
CuF	-327.7	3.396	324.6	1017
CuF_2	-683.4	3.542	527.9	1645
TiO	-66.20	0.3430	839.3	236.5
Ti_2O_3	-124.0	0.4310	1119	373.7
Ti_3O_5	-162.9	0.5060	1199	463.2
TiO_2-R	-233.3	0.6050	1342	602.2
TiO_2	-233.6	0.6050	1342	602.9
TiO_2-A	-239.5	0.6210	1342	618.1
VO	-157.0	0.8140	800.8	539.8
V_2O_3	-272.2	0.9400	1073	789.4
V_3O_5	-334.3	1.040	1151	921.8
VO_2	196.1	-0.5080	1293	-
V_2O_5	-693.3	1.437	1474	1533
CrO_2	-577.5	1.496	1276	1435
Cr_2O_3	-312.8	1.081	1058	897.3

Cr_3O_4	-237.9	0.9250	974.7	719.7
CrO_3	-1171	2.023	1608	2297
MnO_2	-657.3	1.703	1233	1592
Mn_2O_3	-401.3	1.386	1019	1117
MnO	-198.3	1.028	755.6	649.4
Mn_3O_4	-320.5	1.246	937.1	939.4
FeO	-309.8	1.605	746.1	1004
Fe_2O_3	-470.7	1.626	1007	1299
Fe_3O_4	-409.8	1.593	926.1	1190
CoO	-347.0	1.798	715.4	1086
Co_3O_4	-490.3	1.906	890.4	1379
NiO	-349.5	1.811	717.6	1096
CuO	-431.5	2.236	673.9	1283
Cu_2O	-207.6	2.152	374.6	734.7
TiS_2	-475.8	1.233	957.2	945.7
TiS	-168.9	0.8750	670.6	500.2
CrS	-264.6	1.371	637.7	750.3
Cr_2S_3	-574.6	1.985	803.3	1320
MnS	-220.6	1.143	616.1	607.4
MnS_2	-653.0	1.692	900.4	1235
FeS	-338.6	1.755	609.7	924.0
$FeS_{2(marcasite)}$	-721.9	1.871	893.6	1357
$FeS_{2(pyrite)}$	-711.1	1.843	893.6	1337
CoS_2	-732.4	1.898	871.1	1349
Co_3S_4	-423.0	1.644	702.5	977.6
NiS	-359.5	1.863	590.6	954.3
Ni_3S_4	-488.0	1.897	704.5	1130
Ni_3S_2	-222.7	1.731	446.3	692.4
NiS_2	-753.3	1.952	872.8	1390
CuS	-385.4	1.997	560.6	977.7
Cu_2S	-176.4	1.828	336.8	566.3
TiN	115.2	-0.3980	1299	-
VN	62.48	-0.2160	1238	-
CrN	-35.60	0.1230	1218	113.9
Cr_2N	-13.20	0.09100	681.4	52.84
Mn_4N	-5.900	0.08200	344.0	25.75
Mn_5N_2	-20.44	0.1770	531.2	82.44

Fe_4N	-31.22	0.4310	338.7	134.3
Co_3N	-31.52	0.3270	421.4	124.2

Table S11. Calculated EMF (V) of conversion reactions between fluorides and Li, Na, Mg or Al.

Li					Na				
$bLi + 1/a\ M_aX_b = b/aLi_aX + M$					$bNa + 1/a\ M_aX_b = b/aNa_aX + M$				
MX	ΔG (kJ mol^{-1})	EMF (V)	Capacity (+) (mAh g^{-1})	Energy Density (Wh kg^{-1})	MX	ΔG (kJ mol^{-1})	EMF (V)	Capacity (+) (mAh g^{-1})	Energy Density (Wh kg^{-1})
TiF_3	-401.1	1.386	766.8	886.5	TiF_3	-276.9	0.9570	766.8	442.5
TiF_4	-791.8	2.052	865.5	1451	TiF_4	-626.2	1.623	865.5	806.0
VF_3	-536.4	1.853	744.9	1157	VF_3	-412.2	1.424	744.9	647.3
CrF_3	-659.7	2.279	737.7	1412	CrF_3	-535.5	1.850	737.7	835.8
MnF_2	-368.3	1.909	576.8	957.8	MnF_2	-285.5	1.480	576.8	570.9
MnF_3	-763.1	2.636	718.3	1597	MnF_3	-638.9	2.207	718.3	981.0
FeF_2	-506.8	2.626	571.2	1307	FeF_2	-424.0	2.197	571.2	842.3
FeF_3	-791.0	2.733	712.6	1644	FeF_3	-666.9	2.304	712.6	1019
CoF_2	-528.2	2.737	553.0	1324	CoF_2	-445.4	2.308	553.0	865.7
CoF_3	-1044	3.607	693.6	2121	CoF_3	-919.9	3.178	693.6	1382
NiF_2	-571.3	2.961	554.4	1435	NiF_2	-488.5	2.532	554.4	951.1
CuF	-327.7	3.396	324.6	1017	CuF	-286.3	2.967	324.7	753.6
CuF_2	-683.4	3.542	527.9	1645	CuF_2	-600.6	3.112	527.9	1131
Mg					Al				
$b/2\ Mg + 1/a\ M_aX_b = b/2a\ Mg_aX_2 + M$					$b/3\ Al + 1/a\ M_aX_b = b/3a\ Al_aX_3 + M$				
MX	ΔG (kJ mol^{-1})	EMF (V)	Capacity (+) (mAh g^{-1})	Energy Density (Wh kg^{-1})	MX	ΔG (kJ mol^{-1})	EMF (V)	Capacity (+) (mAh g^{-1})	Energy Density (Wh kg^{-1})
TiF_3	-244.7	0.8450	766.8	480.9	TiF_3	-69.10	0.2390	766.8	145.6
TiF_4	-583.2	1.511	865.5	939.3	TiF_4	-349.1	0.9050	865.5	606.8
VF_3	-380.0	1.313	744.9	731.0	VF_3	-204.4	0.7060	744.9	420.9
CrF_3	-503.2	1.739	737.7	961.0	CrF_3	-327.7	1.132	737.7	669.4
MnF_2	-264.0	1.368	576.8	625.5	MnF_2	-147.0	0.7620	576.8	368.0

MnF_3	-606.7	2.096	718.3	1136	MnF_3	-431.1	1.489	718.3	862.0
FeF_2	-402.5	2.086	571.2	946.3	FeF_2	-285.5	1.479	571.2	709.1
FeF_3	-634.7	2.193	712.6	1181	FeF_3	-459.1	1.586	712.6	912.1
CoF_2	-423.9	2.197	553.0	971.3	CoF_2	-306.9	1.590	553.0	741.8
CoF_3	-887.7	3.067	693.6	1618	CoF_3	-712.1	2.460	693.6	1384
NiF_2	-467.0	2.420	554.4	1072	NiF_2	-350.0	1.184	554.4	847.7
CuF	-275.6	2.856	324.7	808.3	CuF	-217.0	2.249	324.7	658.6
CuF_2	-579.1	3.001	527.9	1278	CuF_2	-462.1	2.395	527.9	1074

Table S12. Key elements in the battery assembling and the toxicity.

Elements Abundance& Toxicity					
No.	Atomic Weight	Name	Sym.	Earth crust(%)	Toxicity
14	28.0855	Silicon	Si	27.69	Relatively nontoxic
13	26.9815	Aluminum	Al	8.07	Neurotoxicity (high doses); allergy
26	55.845	Iron	Fe	5.05	Free iron in the cell is detrimental to DNA, proteins, lipids, and other cellular components. 20 milligrams of iron for every kilogram of mass is toxic, and 60 milligrams per kilogram is considered a lethal dose.
11	22.9897	Sodium	Na	2.75	Relatively nontoxic
19	39.0983	Potassium	K	2.58	Relatively nontoxic
12	24.305	Manganese	Mg	2.08	Relatively nontoxic
22	47.867	Titanium	Ti	0.62	Non-toxic
15	30.9738	Phosphorus	P	0.13	White phosphorus is toxic (causing severe liver damage on ingestion
6	12.0107	Carbon	C	0.094	Relatively nontoxic
25	54.938	Manganese	Mn	0.09	Neurotoxicity
24	51.9961	Chromium	Cr	0.035	Acute toxicity; Genotoxicity; Sensitization & irritation; Carcinogenicity
28	58.6934	Nickel	Ni	0.019	Acute toxicity; Genotoxicity; Carcinogenicity; Reproductive toxicity
23	50.9415	Vanadium	V	0.016	Vanadium compounds are toxic
29	63.546	Copper	Cu	0.006	Free copper is toxic, similar to iron
27	58.9332	Cobalt	Co	0.002	Lung toxicity; Genotoxicity; Carcinogenicity
3	6.941	Lithium	Li	0.002	Neurotoxicity (toxic amounts on blood levels >1.5 mmol/l)
50	118.71	Tin	Sn	0.00022	Acute toxicity; Neurotoxicity
51	121.76	Antimony	Sb	0.00002	Antimony and many of its compounds are toxic, similar to arsenic

Figure S1. Capacity values of typical lithium-free cathodes.

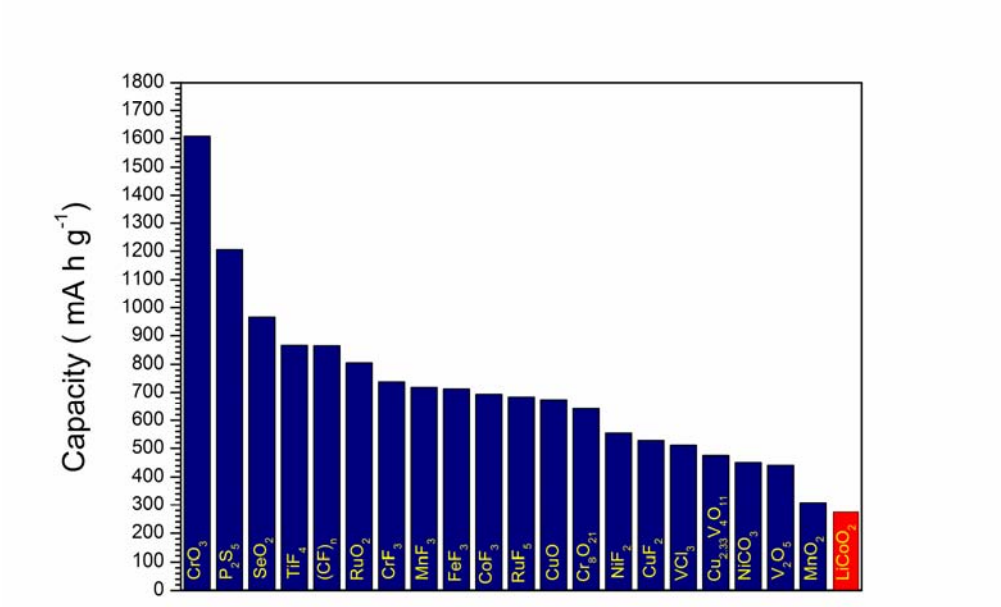


Figure S2. Capacity values of lithium-contained cathodes.

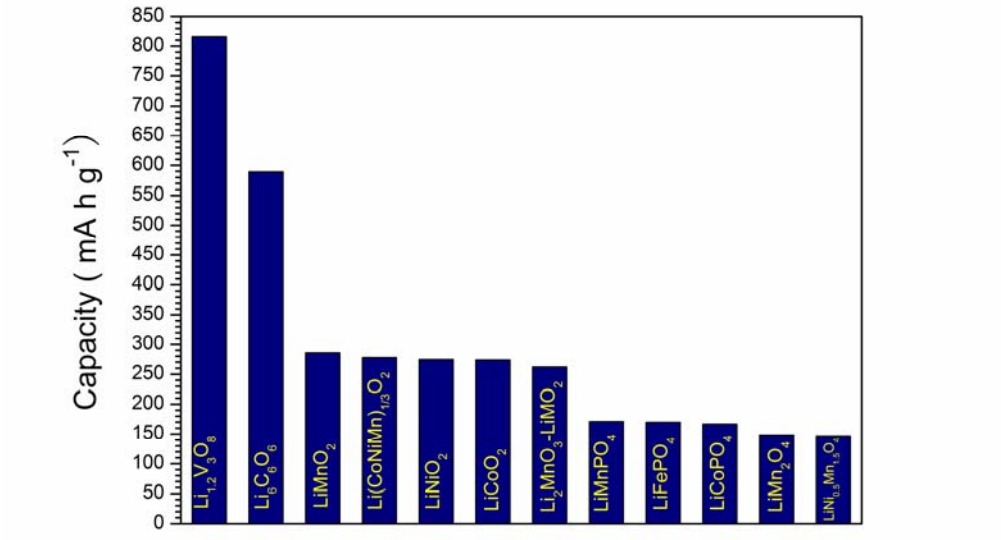


Figure S3. Capacity values of typical anodes.

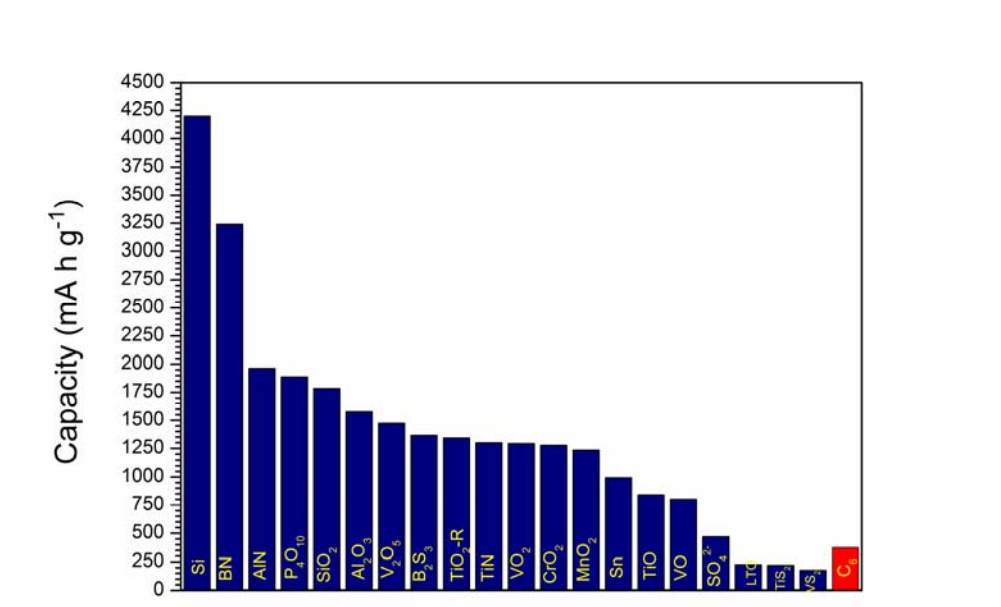


Figure S4. Calculated EMF values (V) of conversion reactions between transition mental salts and lithium.

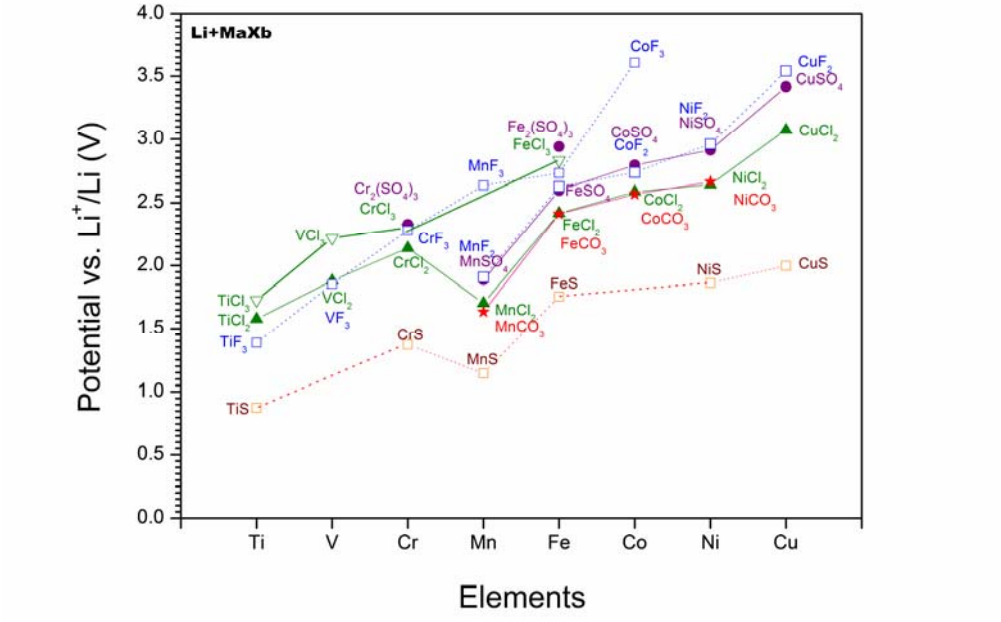


Figure S5. Calculated EMF values (V) of conversion reactions between binary transition mental compounds and sodium.

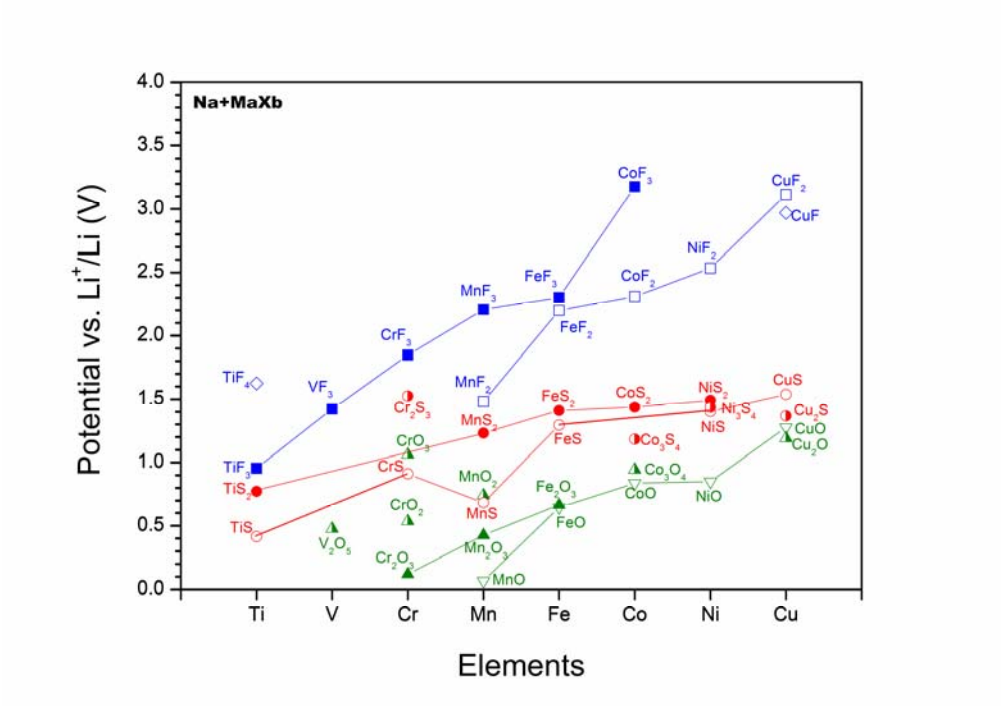


Figure S6. Calculated EMF values (V) of conversion reactions between binary transition mental compounds and magnesium.

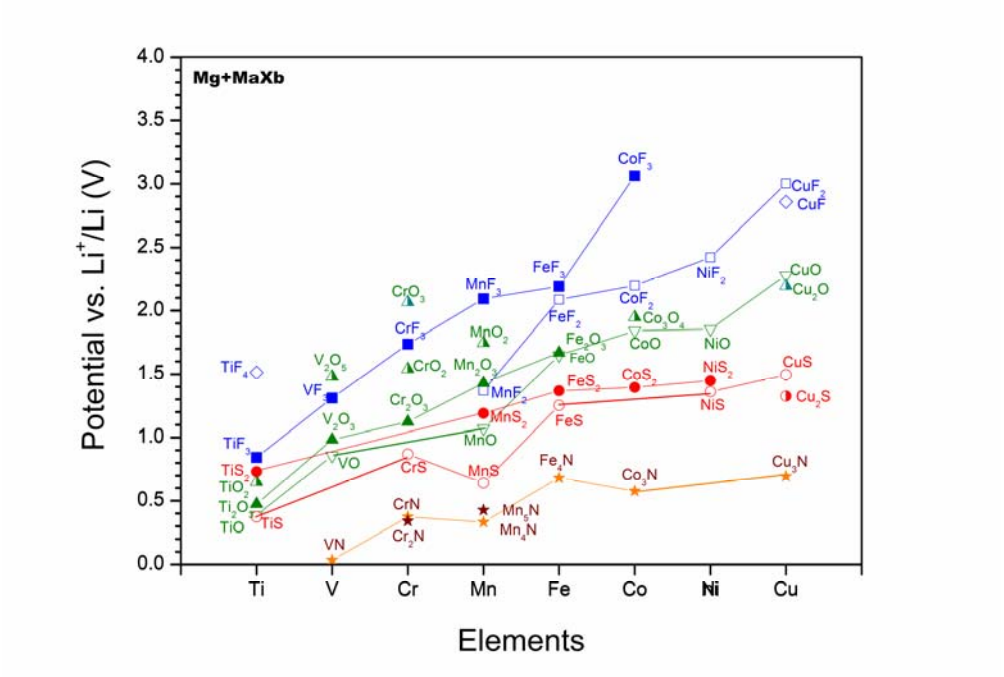


Figure S7. Calculated EMF values (V) of conversion reactions between binary transition mental compounds and aluminum.

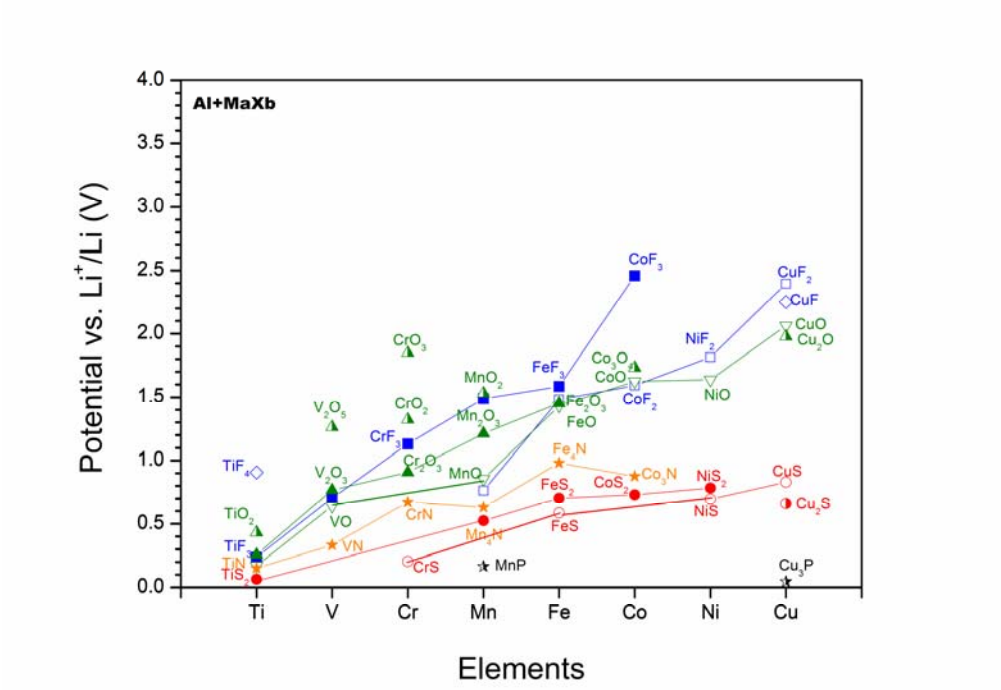


Figure S8. Calculated EMF (V) of conversion reactions between oxides and Li, Na, Mg or Al.

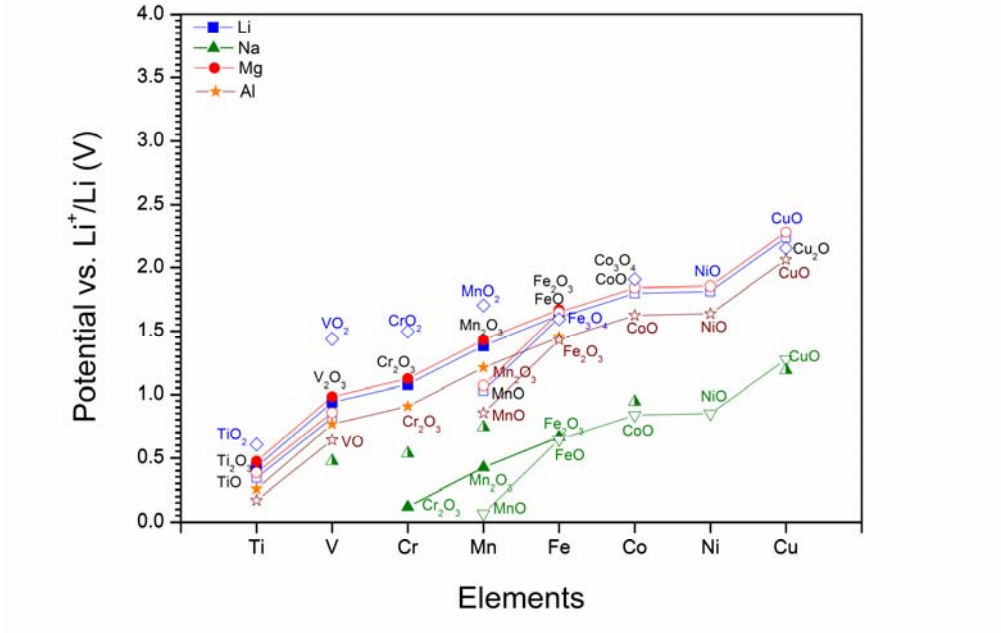


Figure S9. Calculated EMF (V) of conversion reactions between sulphides and Li, Na, Mg or Al.

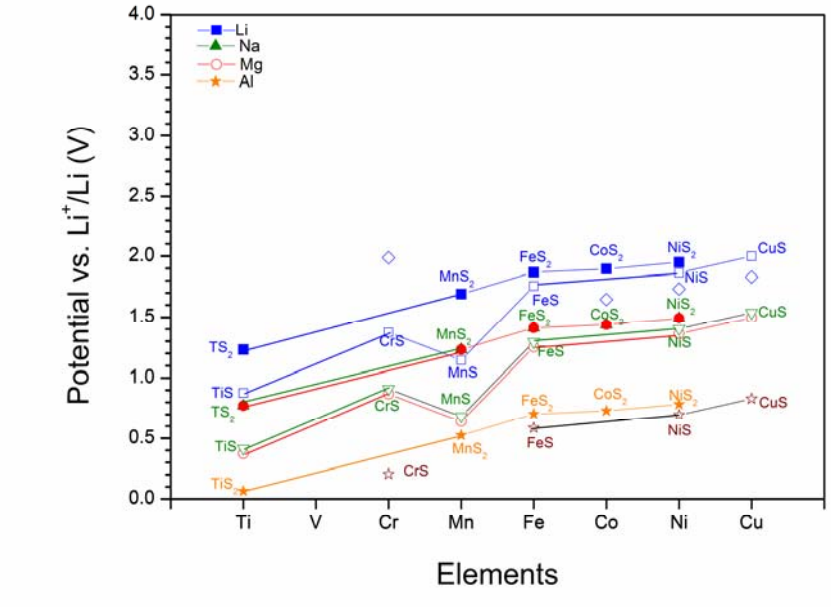


Figure S10. Calculated EMF (V) of conversion reactions between nitrides and Li, Na, Mg or Al.

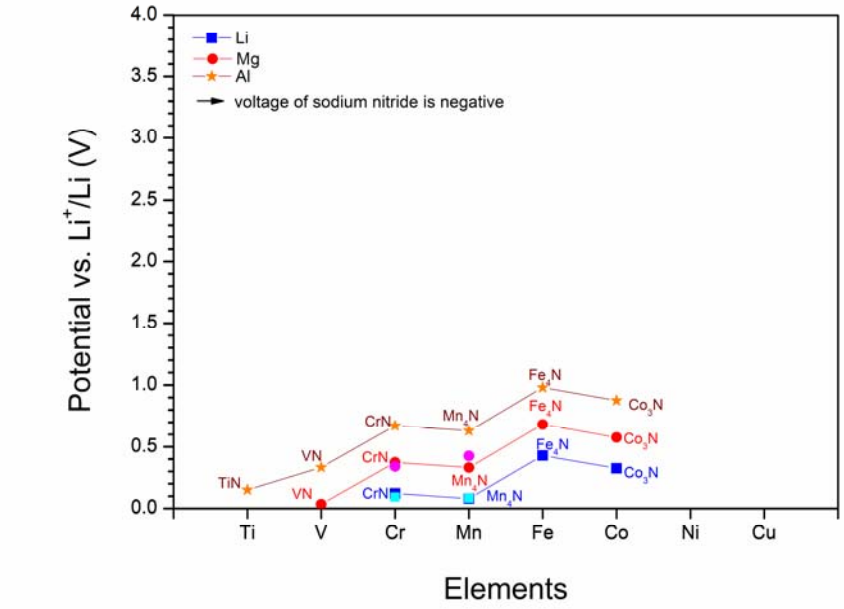


Figure S11. Calculated EMF (V) of conversion reactions between fluorides and Li, Na, Mg or Al.

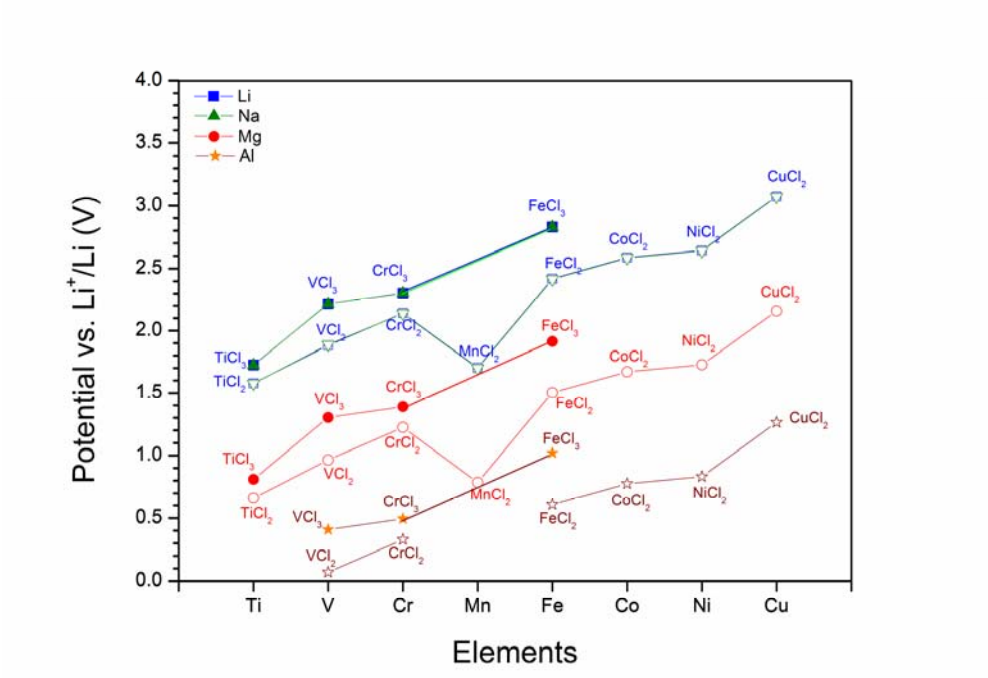
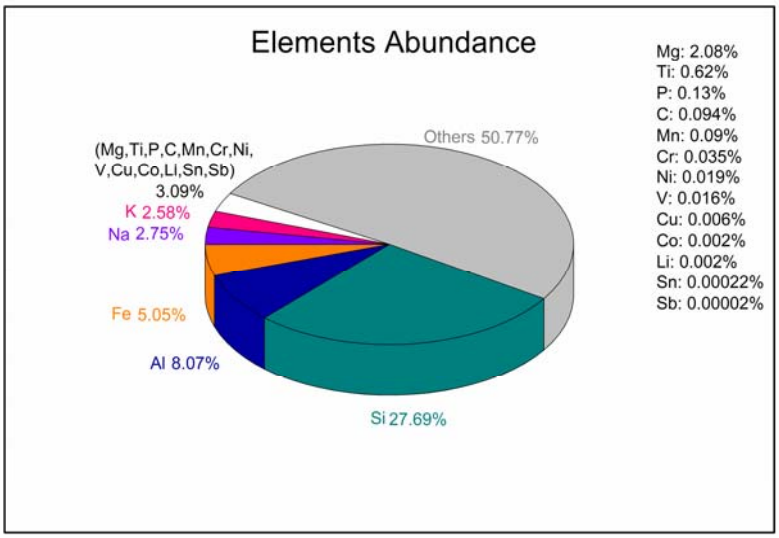


Figure S12. Elements abundance in the earth.



References

1. M. Winter, J. O. Besenhard, M. E. Spahr and P. Novak, *Adv. Mater.*, 1998, **10**, 725-763.
2. G. Q. Liu, L. Wen and Y. M. Liu, *J. Solid State Electrochem.*, 2010, **14**, 2192-2202.
3. M. Broussely, P. Biensanb and B. Simon, *Electrochimica Acta*, 1999, **45**, 3-22.
4. K. L. Huang, Z. X. Wang and S. Q. Liu, *Lithium Ion Batteries Principles and Key Technology*, Chemical industry press, 2007.
5. H. Gwon, D. H. Seo, S. W. Kim, J. Kim and K. Kang, *Adv. Funct. Mater.*, 2009, **19**, 3285.
6. T. F. Yi, Y.R. Zhu and R.S. Zhu, *Solid State Ionics*, 2008, **179**, 2132.
7. Y. Imai and A. Watanabe, *J. Alloys Compd.*, 2007, **439**, 258.
8. P. Limthongkul, Y. Jang, N. J. Dudney and Y. M. Chiang, *Acta Mater.*, 2003, **51**, 1103.
9. C. J. Wen and R. A. Huggins, *J. Electrochem. Soc.*, 1980, **128**,1181.
10. P. Reale, S. Panero, B. Scrosati, J. Garche, M.Wohlfahrt-Mehrens and M. Wacheler, *J. of Electrochem. Soc.*, 2004, **151**, A2138.
11. M. Winter, J. O. Besenhard, M. E. Spahr, and P. Novak, *Adv. Mater.*, 1998, **10**, 725.
12. S. Okada, S. Sawa, M. Egashira, J. Yamaki, M. Tabushi, H. Kageyama,

T. Konishi and A. Yoshino, *J. Power Sources*, 2001, **97-98**, 430.

13. I. Plitz, A. Dupasquier, F. Badway, J. Gural, N. Pereira, A. Gmitter and G. G. Amatucci, *Appl. Phys.*, 2006, **A82**, 615.
14. M. R. Palacín, *Chem. Soc. Rev.*, 2009, **38**, 2565 – 2575.
15. K. Du, Z. Peng, G. Hu, Y. Yang, L.Qi, J. Alloys Compd, 2009. **476**, 329.
16. D. Linden and T. B. Reddy, *Handbook of Batteries 3rd edn.*, 2002 McGraw-Hill.
17. J. G. Zhang, D. Y. Wang, W. Xu, J. Xiao and R. E. Williford, *J. Power Sources*, 2010, **195**, 4332.
18. H. Y. Chen, M. Armand, G. Demailly, F. Dolhem, P. Poizot and J.-M. Tarascon, *ChemSusChem*, 2008, **1**, 348-335.
19. M. Armand, S. Grugeon, H. Vezin, S. Laruelle, P. Ribiere, P.Poizot and J.-M. Tarascon, *Nature Mater.*, 2009, **8**,120.
20. H. Y. Chen, M. Armand, M. Courty, M. Jiang, C. P. Grey, F. Dolhem J.-M. Tarascon and P. Poizot, *J. Am. Chem. Soc.*, 2009, **131**,8984.
21. N.Tran, L. Croguennec, M. Menetrier, F. Weill, Ph. Biensan, C. Jordy and C. Delmas, *Chem. Mater.*, 2008, **20**, 4815.
22. C. S. Johnson, N. Li, C. Lefief, J. T. Vaughey and M. M. Thackeray, *Chem. Mater*., 2008, **20**, 6095.
23. I. Barin and G. Platzki, *Thermochemical Data of Pure Substances*, 3rd.edn, VCH (1995).
24. R. David, *CRC handbook of Chemistry and Physics*, 90 th edn., Boca

Raton. Fla. CRC Press(2009).

25. J. G. Speight, *Lange's handbook of chemistry*, 16th edn. Mc Graw-Hill (2005)B
26. Q. Zha, *Electrochemical power sources*, Wuhan University Press, 2005.
27. Environmental Health Criteria 234-Elemental Speciation in human health risk assessment-World Health Organization.
28. http://en.wikipedia.org
29. *Stabilized spinels and nano olicines*, A. Manthiram, May 2009.

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