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ANALYSIS

Thermodynamic analysis on energy densities of batteries†‡

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The average increase in the rate of the energy density of secondary batteries has been about 3% in the past 60 years. Obviously, a great breakthrough is needed in order to increase the energy density from the current 210 Wh kg^{-1} of Li-ion batteries to the ambitious target of 500–700 Wh kg^{-1} to satisfy application in electrical vehicles. A thermodynamic calculation on the theoretical energy densities of 1172 systems is performed and energy storage mechanisms are discussed, aiming to determine the theoretical and practical limits of storing chemical energy and to screen possible systems. Among all calculated systems, the Li/F_2 battery processes the highest energy density and the Li/O_2 battery ranks as the second highest, theoretically about ten times higher than current Li-ion batteries. In this paper, energy densities of Li-ion batteries and a comparison of Li, Na, Mg, Al, Zn-based batteries, Li-storage capacities of the electrode materials and conversion reactions for energy storage, in addition to resource and environmental concerns, are analyzed.

1. Introduction

Secondary batteries have become a core technology for supporting the development of a sustainable and mobile society. The demand for advanced batteries with high energy densities is increasing continuously due to the rapid progress of wide applications from advanced portable electronic devices to electric vehicles (EVs) and smart grids.[1,2] The importance of the development of secondary batteries has been recognized by governments, and clear targets and roadmaps have been set. For example, the New Energy and Industrial Technology Development Organization (NEDO) in Japan released their project on Li-ion and advanced battery development in 2008. Their targets are 500 Wh kg^{-1} before 2030 and 700 Wh kg^{-1} afterward to develop high-performance, low-cost rechargeable batteries for accelerating the commercialization of new vehicles such as EVs.[3,4]

Can these ambitious targets be realized within the expected duration and can Li-ion batteries take a continuous leading role? An analysis of the battery development in term of energy density, possible energy storage mechanisms and a theoretical thermodynamic calculation on the energy densities of possible batteries and related materials are performed to address these questions.

2. Progress of batteries in term of energy density

Fig. 1 and Fig. 2 present the roadmap of primary and secondary batteries from 1900 to now, respectively. The Zn/MnO_2 (NH_4Cl or $ZnCl_2$) type primary battery dominated almost the whole

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Broader context

Greatly increasing energy densities of current rechargeable batteries has become urgently needed to progress from today's hybrid electric vehicles to plug-in hybrids to all-electric vehicles. This is also essential for many new technologies, such as advanced portable electronic devices, robot and unmanned aerial vehicles. Some battery systems, such as Li-S and Li-air batteries, have been expected to increase the energy densities 2–10 times greater than that of current Li-ion batteries. Are these targets realizable? Can we increase the energy density of Li-ion batteries further? Which system is worthy of being investigated as next generation high energy density battery? Thermodynamic calculation on 1172 material systems has been performed. The calculated energy densities and the voltage of the batteries are reported in this paper. These results are helpful for clarifying above questions and determining the theoretical limit of electrical energy storage in chemical power sources. In addition, concerns about lithium supply due to potential large scale production of batteries for electric vehicles and smart grid are analyzed.

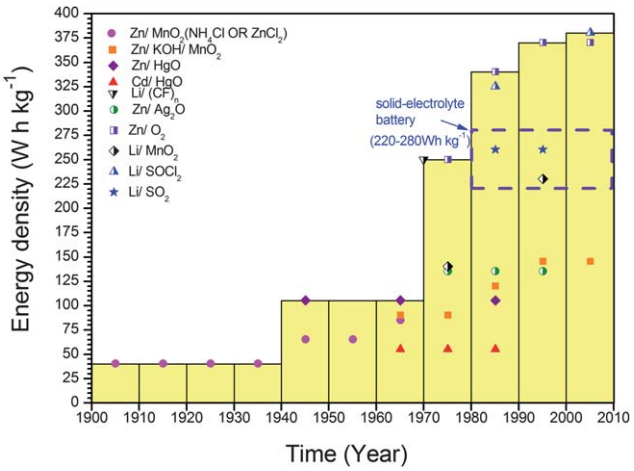


Fig. 1 History of development of primary batteries in view of energy density. Data is taken from literature.[5]

market before the 1940s.[5] In the 1960s, the Zn/KOH/MnO_2 battery took the leading role, pulling the energy density level from 40 Wh kg^{-1} to 100 Wh kg^{-1}. Due to the significant advantage of its low cost, it has been developed continuously and is used widely even today. Primary lithium batteries (Li/MnO_2, Li/$(CF)_n$) and Zn-air batteries appeared around the 1970s. The energy density was doubled to 200–250 Wh kg^{-1}. In the 1980s, primary Li/SO_2 and Li/$SOCl_2$ batteries were applied in special fields and the energy density reached over 380 Wh kg^{-1}. Actually, lithium dry polymer electrolyte batteries have been developed since 1980.[5] Their energy densities ranged from 220–280 Wh kg^{-1}. They have not been commercialized and are still being developed as secondary batteries.

The rechargeable lead-acid battery has been commercialized for more than 100 years. The energy density has increased gradually from initial 25 Wh kg^{-1} to the current 55 Wh kg^{-1}. Although the energy density is not very satisfactory, it is still the main choice for starting, lighting and ignition (SLI) in automobiles and backup battery due to the advantages of high reliability, low cost, moderate power density, acceptable cycling performance and good recycling feature. The nickel-cadmium battery has also been widely used for many small portable electronic devices before the appearance of the nickel metal hydride battery and lithium ion batteries in the 1990s, and because of its environmental impact the market share decreased significantly afterward. In the early 1980s, a rechargeable sodium-sulfur battery was developed. It operates around 300 °C with energy density of 100–150 Wh kg^{-1}. Currently, the Na–S battery is one of the choices as large-scale stationary battery for load-leveling applications.[6] The nickel metal hydride battery appeared on the market in 1989 with energy density of 50–80 Wh kg^{-1}.[7,8] Almost two years later, the Li-ion battery was commercialized by the Sony company.[9,10] The energy density has increased steadily from 90 Wh kg^{-1} to the current 210 Wh kg^{-1}.

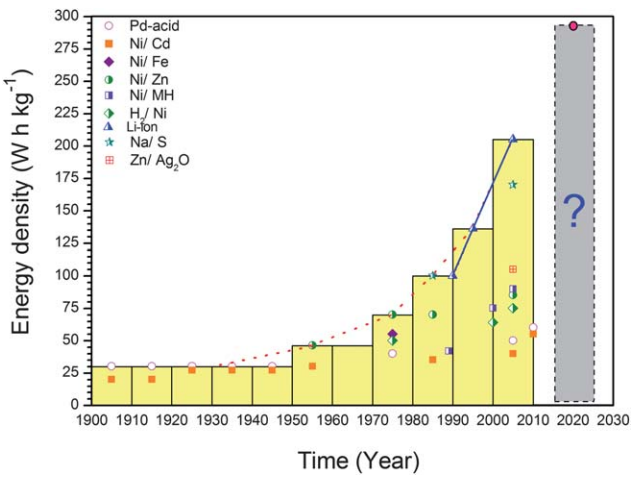


Fig. 2 History of development of secondary batteries in view of energy density. Data is taken from literature.[4] Dash line shows the progress of last 80 years and solid line represents the development of Li-ion batteries in last 20 years.

From 1950 to 2010, the energy density of commercial secondary batteries increased by about 3 Wh kg^{-1} per year in average as shown in the dashed line in Fig. 2. Following this growth rate, the target energy densities of 500 Wh kg^{-1} and 700 Wh kg^{-1} will be realized in years of 2110 and 2177 respectively from the current 210 Wh kg^{-1}. Actually, the annual growth rate from 1990 to 2010 was accelerated to about 5.5 Wh kg^{-1} due to the invention and development of Li-ion batteries, as shown by the solid line in Fig. 2. Based on this, the targets of 500 Wh kg^{-1} and 700 Wh kg^{-1} can be realized in years of 2064 and 2100, respectively. However, it is still far behind the NEDO's target. As shown in Fig. 1 and 2, the growth rate of the energy densities of the batteries is steady for 20–30 year periods until the appearance of the next new technology.

It is essential to estimate the limit of energy densities of possible battery systems for storage and converting chemical energy into electric energy. The theoretical energy density of any battery can be simply calculated from the thermodynamic data once the positive and the negative electrode materials are selected. In addition, the thermodynamic equilibrium voltage (or so-called electronic motive force, in brief, emf) of the battery can be also calculated, as shown below.

3. Calculation formulas

Any chemical reaction which contains two different reactants and in which charge transfer occurs could be applied for electrochemical energy storage.

Such a reaction can be written as:

$$\alpha A + \beta B \rightarrow \gamma C + \delta D \quad (1)$$

Here, the Gibbs free energy of the reaction under standard condition ($\Delta_r G^\ominus$) can be calculated from the sum of the formation energy of the reactants and products:

$$\Delta_r G^\ominus = \gamma \Delta_f G_C^\ominus + \delta \Delta_f G_D^\ominus - \alpha \Delta_f G_A^\ominus - \beta \Delta_f G_B^\ominus \quad (2)$$

If the value of $\Delta_r G^\ominus$ is negative, the electrochemical reaction along the direction defined in the eqn (1) could occur spontaneously and the reaction can be considered for electrochemical energy storage. The maximum electrical work from this reaction equals to $\Delta_r G^\ominus$, as shown in the Nernst equation:

$$\Delta_r G^{\ominus} = -nEF \quad (3)$$

Here n refers to the number of the charge transferred during the reaction per mole reactant, E is the thermodynamic equilibrium voltage or the so-called electromotive force (emf) value and F is the Faraday constant.

Energy density is always expressed either by the gravimetric energy density Wh kg^{-1} or the volumetric energy density (WhL^{-1}). The gravimetric energy density of a battery can be calculated as following:

$$\varepsilon_M = \Delta_r G^{\ominus}/\Sigma M \quad (4)$$

ΣM is the sum of the formula mole weights of the two reactants.

The volumetric energy density (ε_V) of a battery can be calculated as following:

$$\varepsilon_V = \Delta_r G^{\ominus}/\Sigma V_M \quad (5)$$

ΣV_M is the sum of the formula mole volume of the two reactants.

For a given electrode material, the specific energy storage capacity can be calculated from the eqn (6):

$$\text{Capacity} = nF/3.6\ \text{M (mAh g}^{-1}) \quad (6)$$

M refers to the mole weight of the reactant (g mol^{-1}).

Accordingly to the eqn (1 to 5), the theoretical energy density and theoretical voltage can be calculated when the values of the Gibbs formation energy of the reactant and the density of the reactant are known. These values can be found in the thermodynamic data handbook.[11–13] If the Gibbs formation energy of the reactant is not known, it can be obtained through first principles calculations.[14]

4. Reversible energy storage mechanisms

Before discussing the energy density of the battery, it is necessary to summarize possible reaction mechanisms for energy storage. Taking lithium-storage as an example, eight possible reversible lithium storage mechanisms are listed in Fig. 3 and summarized below.

4.1 Intercalation reaction mechanism

An intercalation reaction indicates that guest atoms are accommodated in the structure of the host compounds accompanied by charge transfer:[15–17]

$$xA^+ + xe^- + H \leftrightarrow A_xH \quad (7)$$

A layered structure is preferred for the host compounds, but not limited to this. The "rocking chair concept" for rechargeable lithium batteries, in which the intercalation compounds were suggested to be used in both the positive and negative electrodes, were firstly suggested by Armand in 1972 [18] and commercialized by SONY in 1990.[9,10] In current Li-ion batteries for portable electronic devices, layered structure graphite (R-3m space group) and $LiCoO_2$ (R-3m space group) are used as the negative and the positive electrode material, respectively. Thus, the guest atoms occupy the host lattice continuously and the chemical potential of the host is modified gradually. The voltage profile of charging and discharging within a single-phase intercalation regime normally shows a slope behavior and can be explained by the lattice gas model.[19,20] The reversible lithium storage capacity is determined by the available vacancy sites for guest atoms, a transferrable charge number above 0.0 V *vs.* Li^+/Li and the structure stability of the host. Typically, the reversible lithium storage capacity for the graphite negative electrode is 300–350 mAh g^{-1} (theoretical capacity is 372 mAh g^{-1} for forming LiC_6) and is around 135–145 mAh g^{-1} for the $LiCoO_2$ positive electrode (the theoretical capacity is 274 mAh g^{-1} for extracting one mole of lithium).

4.2 Phase transition mechanism

During discharging or charging, the reactant transforms directly and continuously from the initial phase into another phase. For example, $LiFePO_4$ converts into $FePO_4$ during charging (delithiation)[21] and $Li_4Ti_5O_{12}$ anode converts into $Li_7Ti_5O_{12}$ during discharging (lithiation).[22] In addition, it is also common that the electrode material could undergo a series of phase transitions during continuous lithium insertion or extraction. Taking the alloy-type reaction as an example, Si can form a series of Li–Si alloys during electrochemical lithiation at high temperatures and show several voltage plateaus in the voltage profile.[23]

The open circuit voltage profile of each phase transition reaction will show one plateau when the Gibbs formation energy of the reactants and products do not vary upon lithium insertion and extraction within the phase transition regime.

4.3 Conversion reaction mechanism

The "conversion reaction" is a kind of phase transition mechanism. The term is used here to define specifically the

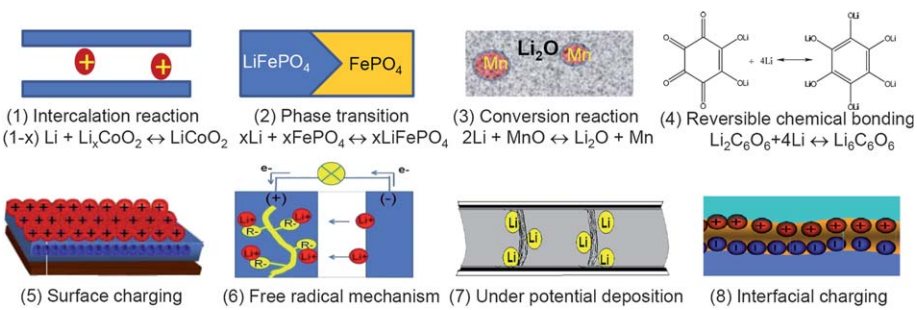


Fig. 3 Scheme of reversible lithium storage mechanisms. See explanation in text part.

decomposition reaction from one parent compound into two or more products after lithium insertion. Reversible heterogeneous conversion reactions of transition metal oxides (TMO) with lithium were reported for the first time on 2000 by Poizot *et al.*:[24]

$$2Li + TMO \leftrightarrow Li_2O + TM\ (TM = Co, Fe, Ni, Cu) \quad (8)$$

Later, reversible lithium storage has been observed in transition metal fluorides, sulfides, nitrides, phosphides and hydrides.[25–29] Recently, the reversible conversion reaction is also extended to other polyanion compounds, such as the reaction (9):[30]

$$xLi + Cu_{2.33}V_4O_{11} \leftrightarrow Li_xV_4O_{11} + 2.33Cu \quad (9)$$

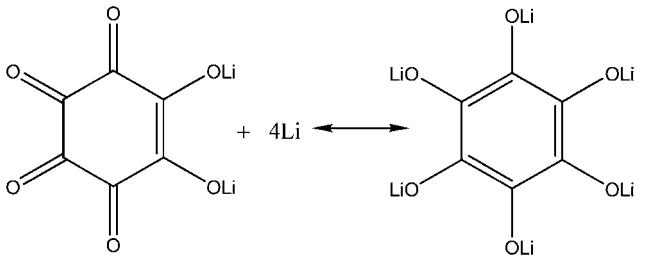
The lithium storage capacity through the conversion reaction can be as high as 1480 mAh g^{-1} in the case of MgH_2 anode for Li batteries (theoretical capacity is 2062 mAh g^{-1} for forming Mg and 2LiH).[29] Many materials undergoing the conversion reaction have been considered as positive or negative electrode materials. In spite of their high capacity, most conversion reaction type electrode materials suffer from high voltage polarization between the charging and discharging, and the low initial Coulombic efficiency.[31–33]

A thermodynamic calculation on the emf value and the Li-storage capacity of dozens of binary compounds was reported in 2004 by Li *et al.*[34] In this paper, a more comprehensive calculation is performed as shown in a later section.

4.4 Reversible chemical bonding

All types of chemical energy storage can be regarded as certain type of reversible chemical bonding. Here this term is used specifically for organic molecules containing carbonyl functional groups, which has been developed recently by scientists in Amiens.[35–38] The carbonyl groups can be utilized to bond with lithium reversibly at room temperature with a reasonable capacity and rate performance.[35–37] A typical compound is dilithium rhodizonate, in which carbonyl groups can be used for lithium storage with a theoretical capacity of 589 mAh g^{-1} at a voltage range of 1.5–3.0 V *vs.* Li^+/Li. This concept has been extended to ethoxycarbonyl-based organic compounds as anode material with a capacity of 100–120 mAh g^{-1} at a voltage range of 1.5–2.0 V. The voltage profiles are plateau type since it is a kind of first-order phase transition reaction. The voltage polarization is much lower than those observed in conversion reactions.[38] Organic electrode materials and the reversible chemical bonding mechanism remain many fundamental issues, such as ion transport, material design and synthesis, stability, as well as technical challenges, such as low volumetric energy density, moderate rate and cyclic performances. However, they are important valuable candidates for a sustainable development of future batteries since they could be produced through biochemistry from abundant natural products.[35–38]

$$Li_2C_6O_6 + 4Li \leftrightarrow Li_6C_6O_6 \quad (10)$$



4.5 Surface charging mechanism

The surface charging mechanism refers to the storage of both anions and cations from the electrolyte on the surface of the two electrodes separately after applying an external electrical field, charge balanced by the holes or electrons within the electrode. Most of the supercapacitors operate based on both the surface charging mechanism in addition to surface redox reactions (pseudo-capacitors).[39–41] The surface charging is related to the occupation of ions at the available surface sites on the surface of the substrate electrode material. Therefore, the voltage profile is a liner shape with a slope of Q/C in a certain voltage range.[42] The capacity of the surface charging is determined by the capacitance, which is related to the surface area, thickness of the double layer, dielectric constant and type of anion and cation in the electrolyte. The supercapacitors have advantages of high rate performance (1–10 kW kg^{-1}) and excellent cyclic performance (~100 000 cycles). Currently, combining the surface charging mechanism and the redox reactions mentioned in 4.1–4.3 has attracted much attention to increase the energy density of supercapacitors.[41]

4.6 Organic free radical mechanism

Organic radical molecules bear one (or multi) unpaired or open-shell electron(s), and they are highly reactive by being converted into closed-shell molecules through a dimer formation or a redox reaction with other molecules, solvents, or molecular oxygen.[43] Radical polymers are aliphatic or non-conjugated polymers which bear organic radicals as pendant groups repetitively in each unit; the outer-sphere redox reactions of the radicals lead to fast electron self-exchange reactions in electrolyte solutions. The large heterogeneous electron-transfer rate of the redox centers and the efficient mass-transfer process within the polymer layers allow facile accommodation of the electrolyte ions to compensate for charges generated from the neutral radicals, in which way the radical polymers serve as ions storage materials, providing an insight into the storage of lithium by forming the corresponding charge pair within the electrode interface.[44] Since the first report on organic radical batteries demonstrated by Nakahara *et al.*,[45] intensive studies have been focused on exploring cathode-active and anode-active materials.[44,46] It was reported that the Li-ion free-radical batteries are superior in safety, sustainability and possess value in the configuration of flexible batteries,[47] however, like organic electrode materials with reversible chemical bonding mechanism, they face intrinsically lower volumetric energy densities.

4.7 Under potential deposition mechanism

It has been proposed that lithium can be stored within the microporous or mesoporous materials just above the plating voltage of lithium at 0.0 V *vs.* Li^+/Li,[48–51] at a form of under potential deposition (UPD). Previous TEM observation has demonstrated the formation and disappearance of lithium clusters within nanopores of carbon nanotubes during discharging and charging.[52] This reaction occurs at lower voltage. Since the formation energy of this reaction is mainly determined by the adsorption energy of lithium on the substrate, related to the occupation of surface sites, the observed voltage profiles are slopes.[53] The kinetic property of lithium storage in microporous materials is not very good.[53] In addition, the deposition voltage is too closed to the plating voltage of lithium, leading to safety concern. Therefore, the UPD mechanism in porous materials is not suitable to be considered for applications in lithium batteries.

4.8 Interfacial charging mechanism

In the study of lithium storage in TiF_3 and VF_3 materials through conversion reaction, it was found that extra lithium can be stored reversibly in the LiF/M nanocomposites at a low voltage range of 0–1.2 V, showing sloped voltage profiles. Since the emf values of the related conversion reactions are higher than 1.2 V *vs.* Li+/Li and both LiF and Ti or V cannot accommodate lithium, it was suggested that this reversible lithium storage mechanism is caused by an interfacial interaction between lithium within the M/LiF matrix, possibly leading to a distinct local charging.[54] A clear physical picture on this phenomenon was given firstly by Jamanik and Maier.[55,56] Further first principles calculation on the lithium storage at the interface between Ti and Li_2O confirmed that this mechanism is thermodynamically favorable.[57] Some experimental evidence of the existence of this type of mechanism has been provided recently.[58,59] The typical lithium storage capacity of the interfacial charging is about 100–300 mAh g^{-1}. The electrochemical potential of the interfacial charging is not very high when a large amount of lithium is inserted into the LiX/M nanocomposite. In view of capacity, Li-storage through interfacial charging is not very competitive compared to other mechanisms for storing lithium in the negative electrode. However, this mechanism should not be ignored when the material has a nanostructure with abundant grain boundaries.

5. Energy density of batteries

5.1 High energy density battery systems

According to the eqn (1 to 5), 1172 reactions have been calculated. The standard Gibbs free enthalpy data and the density data at 25 °C are taken from the literatures.[11–13] The detailed calculated results are provided in the ESI (Table S1).† Fig. 4 displays 20 selected battery systems with higher gravimetric energy densities among all systems. The graphite/$LiCoO_2$ type Li-ion batteries is also included for comparison. Obviously, the reactions show higher energy densities when the formation energy values of the reactants are lower and those of the products are higher. Among all calculated systems, the Li/F_2 battery holds the highest record of 6294 Wh kg^{-1}. The Li/O_2 battery follows

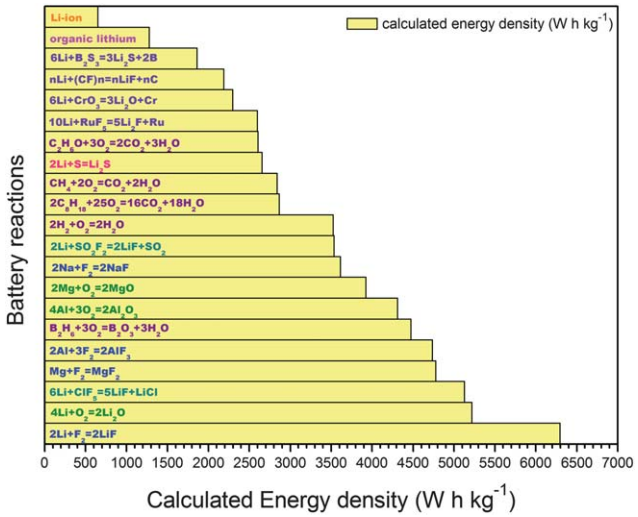


Fig. 4 Calculated energy densities of different battery systems according to the Nernst equation. The formation energies of reactants and products under standard conditions are taken from the literature.[12,13] The energy density of the $Li_2C_6O_6$/Li battery is calculated using data from the literature.[35] Energy densities of the systems containing gas reactants are calculated based on the reaction formula shown in the Figure.

closely with a gravimetric energy density of 5217 Wh kg^{-1}. Besides the reactions of metal with fluorine and oxygen, combustion reactions with oxygen and a few of conversion reactions also show higher energy densities. It has to be mentioned that the combustion reactions can be used to convert chemical energy into the electrical energy directly through fuel cells. The theoretical gravimetric energy densities of these reactions shown in Fig. 4 are calculated for the isolated fuel cell system with stoichiometrical fuel.

5.2 Comparison of batteries using different metal negative electrodes

Fig. 5 shows gravimetric energy densities of selected battery systems using Li, Na, Mg, Al, Zn as the negative electrode,

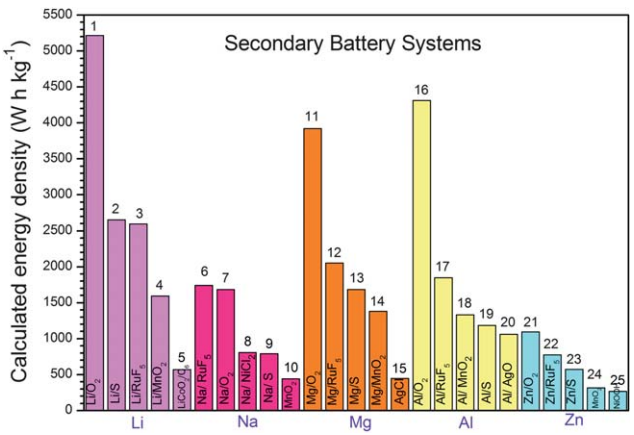


Fig. 5 Comparison of the calculated gravimetric energy densities of different battery systems using Li, Na, Mg, Al or Zn as anodes. The corresponding reactions, emf values and volumetric energy densities are listed in Table 1.

Table 1 Calculated energy densities of different battery systems using Li, Na, Mg, Al or Zn as anodes. The volumetric energy densities of the batteries containing gas components are not calculated

No.	Electrochemical reaction	ΔG/kJ mol^{-1}	EMF/V	Cathode capacity/mAh g^{-1}	Energy density/Wh kg^{-1}	Energy density/W h L^{-1}
1	$4Li + O_2 \leftrightarrow 2Li_2O$	−1122	2.910	3350	5217	—
2	$2Li + S \leftrightarrow Li_2S$	−439.0	2.275	1672	2654	2856
3	$5Li + RuF_5 \leftrightarrow 5LiF + Ru$	−2157	4.472	683.5	2597	5199
4	$4Li + MnO_2 \leftrightarrow 2Li_2O + Mn$	−657.3	1.703	1233	1592	2642
5	$CoO_2 + LiC_6 \leftrightarrow LiCoO_2 + C_6$	−347.4	3.600	273.8	567.8	1901
6	$5Na + RuF_5 \leftrightarrow 5NaF + Ru$	−1950	4.043	683.5	1742	3210
7	$4Na + O_2 \leftrightarrow 2Na_2O$	−751.0	1.950	3350	1683	—
8	$NiCl_2 + 2Na \leftrightarrow Ni + 2NaCl$	−509.2	2.640	413.6	805.6	1677
9	$2Na + 3S \leftrightarrow Na_2S_3$	−405.2	2.100	558.4	791.7	1179
10	$4Na + MnO_2 \leftrightarrow 2Na_2O + Mn$	−285.9	0.741	1233	443.9	709.6
11	$2Mg + O_2 \leftrightarrow 2MgO$	−1139	2.950	3350	3924	—
12	$5/2Mg + RuF_5 \leftrightarrow 5/2MgF_2 + Ru$	−1896	3.931	683.5	2051	6181
13	$Mg + S \leftrightarrow MgS$	−341.8	1.771	1672	1684	3221
14	$2Mg + MnO_2 \leftrightarrow 2MgO + Mn$	−673.5	1.745	1233	1380	4150
15	$Mg + 2AgCl \leftrightarrow MgCl_{2(aq)} + 2Ag$	−497.5	2.580	186.8	444.4	2109
16	$4/3Al + O_2 \leftrightarrow 2/3Al_2O_3$	−1055	2.733	3350	4311	—
17	$5/3Al + RuF_5 \leftrightarrow 5/3AlF_3 + Ru$	−1604	3.325	683.5	1848	6658
18	$4/3Al + MnO_2 \leftrightarrow 2/3Al_2O_3 + Mn$	−589.8	1.528	1233	1333	5384
19	$2/3Al + S \leftrightarrow 1/3Al_2S_3$	−213.3	1.106	1672	1184	2676
20	$2/3Al + AgO \leftrightarrow 1/3Al_2O_3 + Ag$	−541.3	2.805	432.7	1060	6488
21	$Zn + 1/2O_2 \leftrightarrow ZnO$	−320.5	1.660	3350	1094	—
22	$5/2Zn + RuF_5 \leftrightarrow 5/2ZnF_2 + Ru$	−1002	2.077	683.5	776.0	3804
23	$Zn + S \leftrightarrow ZnS$(sphalerite)	−201.3	1.043	1672	573.6	2162
24	$Zn + 2MnO_2 \leftrightarrow ZnO + Mn_2O_3$	−271.4	1.410	308.3	315.1	1738
25	$2NiOOH + 2H_2O + Zn \leftrightarrow 2Ni(OH)_2 + Zn(OH)_2$	−273.0	1.410	292.3	266.2	891.8

respectively. Theoretically, the reaction with fluorine inherits the highest energy density. Since fluorine based batteries seem impossible to be handled, the reactions with oxygen are employed to represent the highest energy density level in each group. Besides, several systems with high energy densities for each metal are selected. For reactions in the same type, lithium battery processes the higher gravimetric energy densities compared to other metal negative electrode systems. However, in terms of volumetric energy density, some Al and Mg systems show certain advantages, as listed in Table 1. As we discussed in the last section, if the production of lithium-based batteries increases rapidly and the recycling technology of the lithium batteries has not been developed very well, the available resources of lithium could be a problem. If this happens, Na, Mg and Al-based rechargeable batteries could be also considered since their theoretical energy densities are comparable to or not too much lower than those of lithium-based systems. Continuous efforts on these batteries have been made.[60–68]

5.3 Energy densities of rechargeable metal lithium batteries

Rechargeable metal lithium batteries have been developed for over 50 years. The dendrite formation of lithium during the charging process was regarded as inevitable. It causes practical problems, such as poor safety characteristics, poor cyclability, and the requirement for a long charging time.[10,69] Up to now, rechargeable lithium batteries have not been commercialized successfully. However, it is believed that those problems could be solved by modifying the surface, replacing the electrolyte or optimizing the electrode and battery structure. When metal lithium is used as the negative electrode, the choice of the positive electrode material can be extended widely from lithium-containing compounds used in Li-ion batteries. The 20 systems with higher energy densities among calculated systems are shown in Fig. 6 for reference (see more results in the ESI: Table S3–S4†).

5.4 Energy densities of Li-ion batteries

Currently, at least three types of Li-ion batteries have been developed for different applications. (1) High energy density (150–210 Wh kg^{-1}): $LiCoO_2$ or $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ is used in

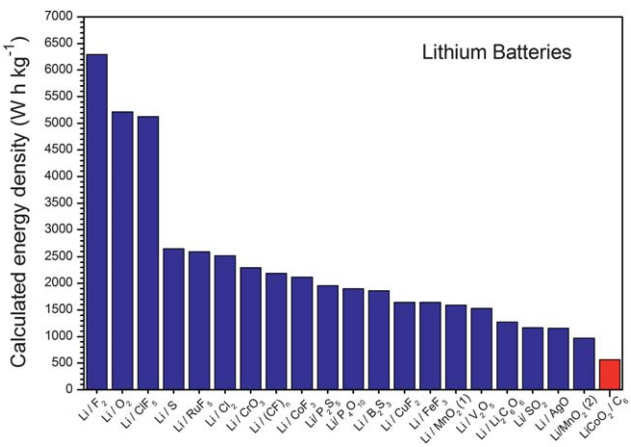


Fig. 6 Comparison of the calculated energy densities of lithium battery systems. Li-ion battery ($LiCoO_2$/C) marked in red is also drawn for comparison. The corresponding reactions are listed in Table S4.† Here Li/MnO_2 (1) refers to conversion mechanism (Li_2O/Mn as product) while Li/MnO_2 (2) refers to intercalation mechanism ($LiMnO_2$ as product).

the positive electrode and graphite is used in the negative electrode. (2) High power density (1000–4000 Wkg^{-1}): $LiMn_2O_4$ or $LiFePO_4$ is used in the positive electrode and graphite or hard carbon is used in the negative electrode. The energy density ranges from 70–140 Wh kg^{-1}. (3) Long cycle life (3000–10 000 cycles of 100% DOD): $LiFePO_4$ is used in the positive electrode and $Li_4Ti_5O_{12}$ or graphite is used in the negative electrode. In order to increase the energy density of Li-ion batteries, high voltage positive electrode materials and high capacity positive and negative materials are pursued. Many materials have been investigated. It seems that Si and lithium-rich compounds are quite competitive as the candidate for the negative and positive electrode respectively. Due to difficulty in finding thermodynamic data of lithium-containing compounds, the theoretical energy densities of Li-ion batteries could be calculated based on the calculated open circuit voltage values (OCV) from literatures and the highest transferable charge number using the eqn (3). Taking the $LiCoO_2/C_6$ as an example, when the OCV is taken as 4.2 V, and charge is taken as one electron. Then calculated value is 648.23 Wh kg^{-1}. However, in the cases that the OCV of the batteries varies with the amount of inserted/extracted lithium, taking average open circuit voltage should be more reasonable. For example, if 3.6 V is taken as the average open circuit voltage (AOCV) for the $LiCoO_2/C_6$ battery, the calculated value is 567.8 Wh kg^{-1} for extracting one lithium. Actually, only 0.5 Li can be extracted. Accordingly, the theoretical energy density of $LiCoO_2/C_6$ battery should be 360 Wh kg^{-1}. It is difficult to calculate or measure average open circuit voltage accurately, therefore, the calculated values of the energy densities using AOCV could be overestimated or underestimated about 8–10% for the intercalation type Li-ion batteries due to the deviation of the average open circuit voltage. In this manuscript, the estimated theoretical energy densities of Li-ion batteries are calculated using AOCV if not mentioned specifically. All calculated results and the parameters can be found in the ESI (Tables S1 & S5).† A comparison of the calculated theoretical gravimetric and volumetric energy density between different materials is also shown in Fig. 7. Among them, the highest value is 963.7 Wh kg^{-1}, which is 267% of the theoretical value of current graphite/$LiCoO_2$ Li-ion batteries.

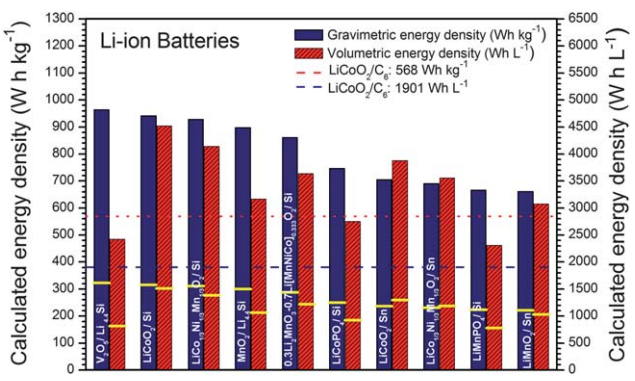


Fig. 7 Comparison of the calculated gravimetric and volumetric energy densities of selected Li-ion batteries. Solid short bar refers to estimated practical energy densities, which are calculated from 1/3 theoretical energy densities.

5.5 Real energy density of typical batteries

Since the weight or volume of the active material for storing chemical energy is only a part of the total weight or volume of the batteries, the real energy densities is always much lower than calculated values. As seen in Table 2, the ratio of the real energy density to calculated energy density (R) is 42–58% for Li-ion batteries. Panasonic announced recently that their Li-ion batteries using Ni-based positive electrode material and Si-based negative electrode material could achieve an energy density of 251.9 Wh kg^{-1} (800 Wh L^{-1}), which is 41.9 Wh kg^{-1} higher than the graphite/$LiCoO_2$ Li-ion batteries.[70]

Taking the highet R value of 58%, the estimated energy density of the Li-ion battery using high capacity materials (Si, $Li_{1.3}Ni_{0.23}Co_{0.23}Mn_{0.54}O_2$), Li-air battery and Li–S battery is approximately 497 Wh kg^{-1}, 3264 Wh kg^{-1} and 1541Wh kg^{-1} respectively. Obviously, it may be not possible for these new batteries to achieve the same R value of 58%. It has to be mentioned that above consideration is suitable for the batteries in which the positive and negative electrode materials are sealed in the container. If the reactants are fed continuously from external sources, as in the fuel cell, or the volume and weight ratio of the reactants are very high, as in the redox flow batteries, this R ratio may be higher, although current technologies show still lower values as listed in Table 2. Typical energy densities of portable fuel cell are claimed at a range of 120–800 Wh kg^{-1} and 110–380 Wh L^{-1}.[71] R values are ranged from 3–23%.

6. Li-storage capacity of the electrode materials

As discussed in the Section 3, the calculated energy density of a battery is determined by the formation energy of the reactants and products. The real energy density equals roughly to the product of the real lithium storage capacity and the average working voltage. The working voltage of a battery is a voltage difference between the electrode potentials of the positive and negative electrode. For Li-ion batteries, in order to achieve high energy density, the average lithium insertion potential of the negative electrode should be as low as possible, just above the lithium plating potential (−50 mV–0 V *vs.* Li$^+$/Li). This requirement is not a problem for most of the high capacity negative electrode materials. The average lithium insertion potential of the positive electrode should be as high as possible, but 0.5–1.0 V below the decomposition potential of nonaqueous organic electrolytes (typically, 4.5–5.0 V *vs.* Li$^+$/Li). The electrode potential at equilibrium state is related to the Fermi level (electrochemical potential) of the active electrode material. It can be calculated simply from the thermodynamic data using the Nernst equation for the phase transition reaction, conversion reaction and chemical bonding reaction as mentioned above. For the intercalation reaction, the estimation of the potential could be obtained through the first principle simulation.[14,72]

The theoretical lithium storage capacity is determined simply by the number of transferable charges and number of extractable or pluggable lithium ions. The real number of pluggable lithium ions is sometimes limited by the structure stability, which is quite difficult to be predicted accurately by theory. Actually, it is very simple to estimate the maximum number of transferable charges. Taking $LiCoO_2$ as an example, Co^{3+} can be oxidized to Co^{4+}.

Table 2 Real energy density of typical batteries

Battery type	Electrochemical reaction	Cal. energy density/Wh kg^{-1}	Real energy density/Wh kg^{-1}	Real/Cal. (%)
Pb-acid	$Pb + PbO_2 + 2H_2SO_4 \leftrightarrow 2PbSO_4 + 2H_2O$	171	25–55	15–32
Na–S	$2Na + 3S \leftrightarrow Na_2S_3$	792	80–150	10–19
Ni-MxH	$1/5LaNi_5(1/2H_2)+NiOOH = Ni(OH)_2 + LaNi_5$	240	50–70	20–29
Li-ion	$2Li_{0.5}CoO_2 + LiC_6 \leftrightarrow 2LiCoO_2 + C_6$	360	150–210	42–58
Li–S	$Li + 2S \leftrightarrow Li_2S$	2654	250–350	9–13
Li-MnO_2	$2Li + 2MnO_2 \leftrightarrow Li_2O + Mn_2O_3$	970	100–220	10–23
Zn–O_2	$Zn + 1/2O_2 \rightarrow ZnO$	1094	150–200	14–18
Li-$(CF)_n$	$Li+(CF)_n \rightarrow LiF + C$	2189	200–300	9–13
Li–O_2	$2Li + O_2 \rightarrow 2Li_2O$	5217	—	—
Li–F_2	$2Li + F_2 \rightarrow 2LiF$	6294	—	—
H_2–O_2	$H_2 + 1/2O_2 \rightarrow H_2O$	3525	120–800	3–23

Therefore, the theoretical capacity can be calculated based on one charge transfer since one mole of lithium is also available. For conversion reaction, taking MnO as an example, Mn^{2+} can be reduced maximally to Mn^0. Two electrons per mole can be transferred. Obviously, multi-electron reaction materials are interest for high capacity materials.[73]

The charge transfer is considered mainly from the valence variable transition metal cations. This is not necessary for all the cases. Sometimes, anions could also take part into redox reactions, such as S in Li–S battery and probably O in lithium-enriched compounds $[xLi_2MnO_3\cdot(1 - x)LiMO_2]$.[74] Charge transfer contributed from both transitional metal and anions could lead to breakthrough of new high capacity cathode materials for Li-ion batteries.

Lithium storage capacities of 448 kinds of materials have been calculated. The detailed results can be found in the ESI (Table S6–S9 and Figure S1–S3).† Apparently, materials undergoing the conversion reaction show a high capacity for the positive electrode materials and the materials undergoing an alloy type reaction show a high capacity for the negative electrode materials.

7. Storing energy through the conversion reaction

The conversion reaction mechanism was introduced in section 4.3. Actually, primary batteries operating through the conversion reaction have been around for a long time, such as the commercialized Li/CuO, Li/$(CF)_n$, Li/SO_2, Li/$SOCl_2$, Li/FeS_2 batteries in the 1980s.[5] However, reversible conversion reactions have attracted wide attention only after the report by P. Pozoit *et al.* in 2000.[24]

Conversion reactions show high voltage hysteresis between the charging and discharging, which is related to both thermodynamic and kinetic factors.[33] The initial Coulombic efficiency is normally less than 75% except for RuO_2.[75] As high capacity negative electrode materials, the materials storing lithium through conversion reactions are not competitive compared to alloy-type materials, in term of high capacity, low voltage and low voltage polarization.

The conversion reaction seems more attractive for exploring the positive electrode materials. The emf values of the binary transitional metal compounds for the same metal with the same valence, have the following order for storing lithium: fluoride > oxide > sulfide > nitride > phosphide. The materials with higher oxidation state show higher emf values. For the same material but inserted by different atoms, the emf values of the conversion reactions for fluorides show the order of Li > Na > Mg >Al. The insertion reactions of Na, Mg and Al are much less studied than the lithium insertion reactions.

These tendencies can be seen clearly in Fig. 8, Fig. 9 and Table S10–S11,† which could be also relevant and helpful to understand the tendency for the materials storing chemical energy through the intercalation or phase transition mechanisms. A comprehensive calculation result can be found in the ESI (Table S1, Figure S4–S11)† for reference.

Two points are worth mentioning. (1) The reversible conversion reaction is a reminder that disordered nanostructured or nanocomposite materials could be also considered as electrode materials, instead of just highly ordered crystalline materials. (2) It is known that the materials cannot be inserted with lithium to complete the conversion reaction if their emf values are less than 0.5–1.0 V *vs.* Li^+/Li due to the high overpotential.[34] This information is helpful for searching solid electrolytes and solid sealant materials for solid state lithium batteries.

8. Resource and environmental issue

Due to the large scale applications and the potential markets for high energy density and high power density batteries for electric

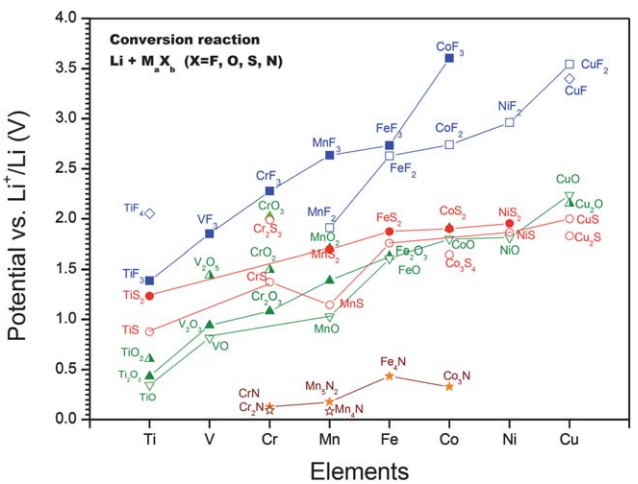


Fig. 8 Calculated EMF values (V) of conversion reactions between selected binary transition metal compounds and lithium.

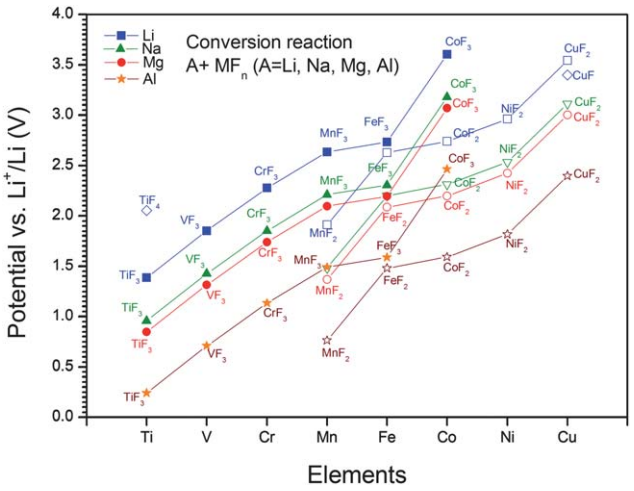


Fig. 9 Calculated EMF (V) of conversion reactions between selected binary transitonal metal fluorides and Li, Na, Mg or Al.

vehicles and long life stationary batteries for smart grid and dispersed renewable energy systems, concerns about the natural resources for the sustainable development of lithium batteries are increasing continuously. The abundance of lithium in earth accounts for only 0.002% among all constituting elements (Figure S12†),[76–78] and only few of countries, such as Argentina, Chile, China, and the United States, are the leading producers of lithium carbonate.[79] According to data from the US Geological Survey (USGS) and Meridian International Research (MIR),[79–82] the resources of lithium are identified as a total of 25.5 million tons 2010, in which the reserve base accounts for approximately 11 million tons and the reserve 4 million tons. Lithium consumption increased by 6% on average per year from 2000 to 2008,[80] from this point it slowed down to less than 4% growth rate owing to the economic crisis.[83] In that time the total world lithium consumption was about 21 280 tons, so the existing resources of lithium could be sustained for approximately 65 years from now on taking an average 5% growth per year as an estimate. (Data of the lithium reserve base are used for estimation and the ever increasing demand from the EV market is not considered at this moment.)

However, the potential market for electrical vehicles could accelerate the demanding for lithium resource to a large scale. Currently, global lithium end-use markets are estimated as follows: ceramics and glass, 31%; batteries, 23%; lubricating greases, 10%; air treatment, 5%; continuous casting, 4%; primary aluminium production, 3%; and other uses, 24%.[80] Lithium use in batteries expanded notably in recent years (20% average growth),[79] and electric vehicle batteries could be projected to dominate the long-term lithium demand. Today, some 60 M light-duty vehicles are produced each year in the world, and in 2050 the number is estimated to be 175 M following a linear growth model.[84] Assuming that around 60% of them might have electric drives and among which EV sales account approximately 22% (an optimistic market penetration scenario is chosen), then if one EV vehicle is equipped with a 50 kWh battery the total lithium request in this aspect alone could be 570 000 t. (existing LiIon/LiMP "Energy Batteries" for EVs require about 0.3 g of lithium metal equivalent per kWh, in the form of lithium carbonate),[81] more than 20 times the current lithium annual world production level of 25 000 t. In terms of the remaining 68 M plug-in hybrid electric vehicle (PHEV) sales, if they were all PHEV 20s with a small 5 kWh battery, the total amount of lithium metals required would therefore be 102 000 t. Actually, according to this model, given that all the lithium reserves were used to satisfy the EV and HEV markets, it would be approximately 36 years before we run out of lithium. In practice, the demand for lithium varies greatly for different types of battery chemistry and the difference could be 5 to 8 times the present energy density level of Li-ion batteries.

World demand for lithium resources, especially in the electric vehicle market is difficult to estimate due to the complex scenarios considering many possible compromises between cost and performance. However, it is safe to say that the new and increasing demand on the lithium supply could be reduced by developing recycling technologies, although currently this contribution is negligible according to the survey from USGS.[80] Since Scrosati *et al.* reported a preliminary laboratory-scale lithium battery recycling process in 1999,[85,86] many endeavors have been made. However, lithium recycling is currently not profitable for small lithium batteries. Obviously, a breakthrough is needed to maximize recovery with minimum impact and decrease the cost. Recently, the ionothermal synthesis method and hydrometallurgical leaching process may possess some value regarding this issue.[87,88] It could be more cost-effective for the recycling of large size battery. It has been estimated that switching from virgin resource supply to recycling for cobalt and nickel for Li-ion battery cathode material results in a 51% natural resource saving.[89]

Table S12 (ESI†) gives toxicity information on major elements that are used in battery assembly. It has been analyzed that the mean cobalt level of the battery electrode is about 45 times the toxicity threshold limit concentration for cobalt while the mean nickel result is about 38 times the toxicity threshold limit concentration. Spent portable rechargeable lithium batteries should be handled as toxic materials that require special treatment. Implementation of a well-coordinated management strategy for spent batteries is urgently required to check the dissipation of large doses of toxic heavy metals into the environment.[90] It should be also mentioned that although chromium and vanadium containing battery systems could deliver higher energy densities, they should not be applied in term of environmental protection due to their high toxicity.

Due to superior recycling technologies, sustainability and green chemistry concepts, organic electrode materials have been studied over the years. The feasibility of using active $Li_xC_6O_6$ organic molecules that could be prepared from natural sugars common to living systems is currently under investigation.[35] Although organic materials have several disadvantages in terms of their limited thermal stability, low specific gravity and poor solubility in electrolytes, the search for electroactive organic molecules synthesized from biomass may pave the way for sustainable development of next generation batteries.[1]

9. Summary and outlook

In the past 60 years, the energy density of rechargeable batteries has increased from 25 Wh kg^{-1} to the current value of

210 Wh kg^{-1}. According to this growth speed, it is not possible to realize the target of 500 Wh kg^{-1} for the application of electric vehicles before the year 2030. A breakthrough is needed urgently. The thermodynamic calculations are helpful for checking the theoretical limitation, predicting and searching possible energy storage systems. It is found that the energy density of the Li/F_2 battery is the highest among calculated 1172 systems. The Li/O_2 battery ranks as No. 2 with a theoretical energy density of 5216.9 Wh kg^{-1}. Currently, the highest ratio of the real energy density to the theoretical energy density is 58%, achieved by the $LiCoO_2/C_6$ Li-ion batteries. If this R value could be hold for many new batteries as calculated in this manuscript, it is really possible to realize the ambitious target of 500–700 Wh kg^{-1}.

Due to the great demand for applications of electric vehicles and stationary batteries for load-leveling and dispersed renewable energy systems, increasing the energy densities and cyclic performance of the batteries, improving the recycling technologies for rechargeable lithium batteries, and developing Na, Mg and Al-based batteries, in addition to organic rechargeable batteries, should be important strategies for sustainable development of secondary batteries. However, many scientific and technological barriers need to be overcome.

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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.

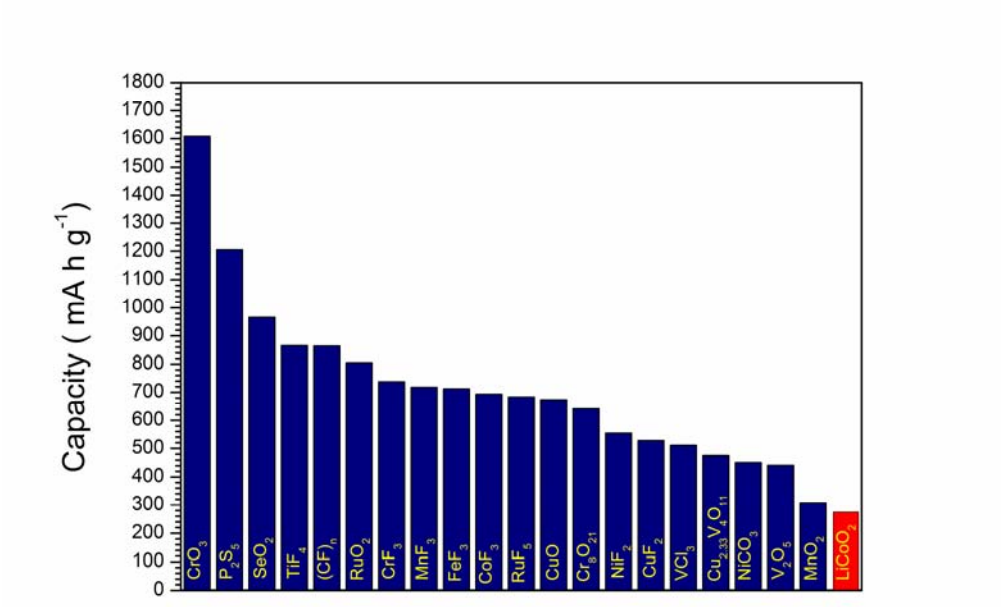


Figure S2. Capacity values of lithium-contained cathodes.

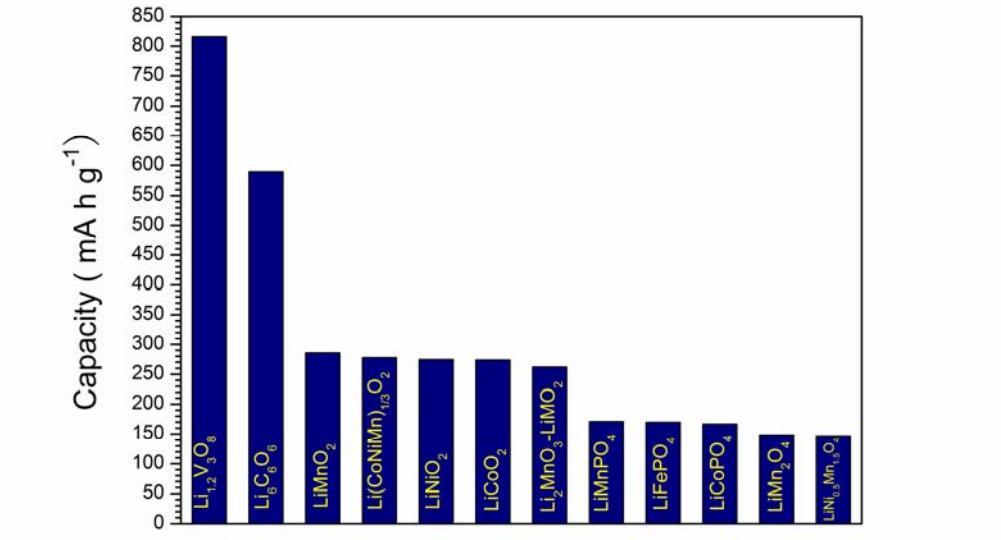


Figure S3. Capacity values of typical anodes.

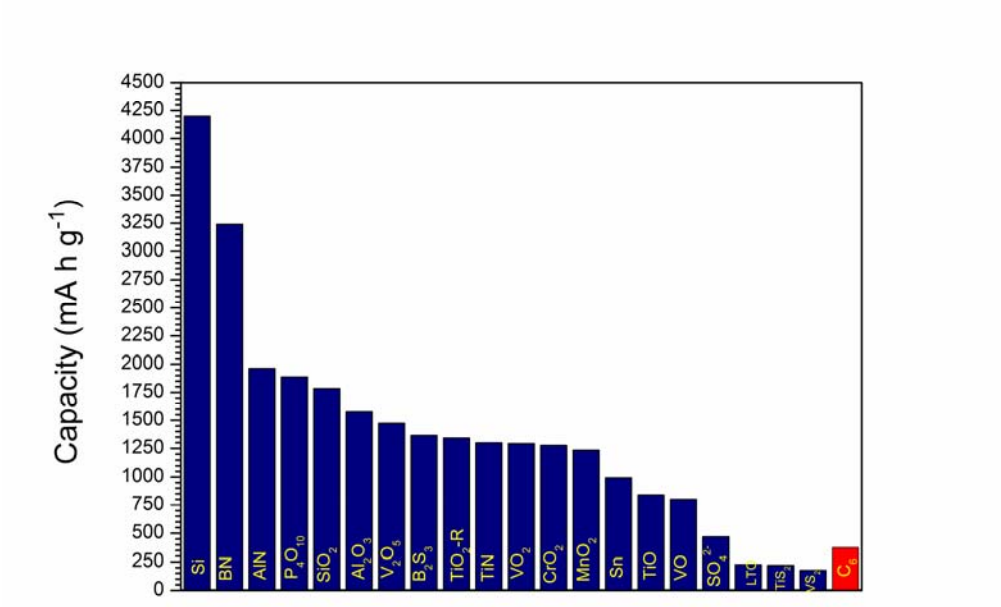


Figure S4. Calculated EMF values (V) of conversion reactions between transition mental salts and lithium.

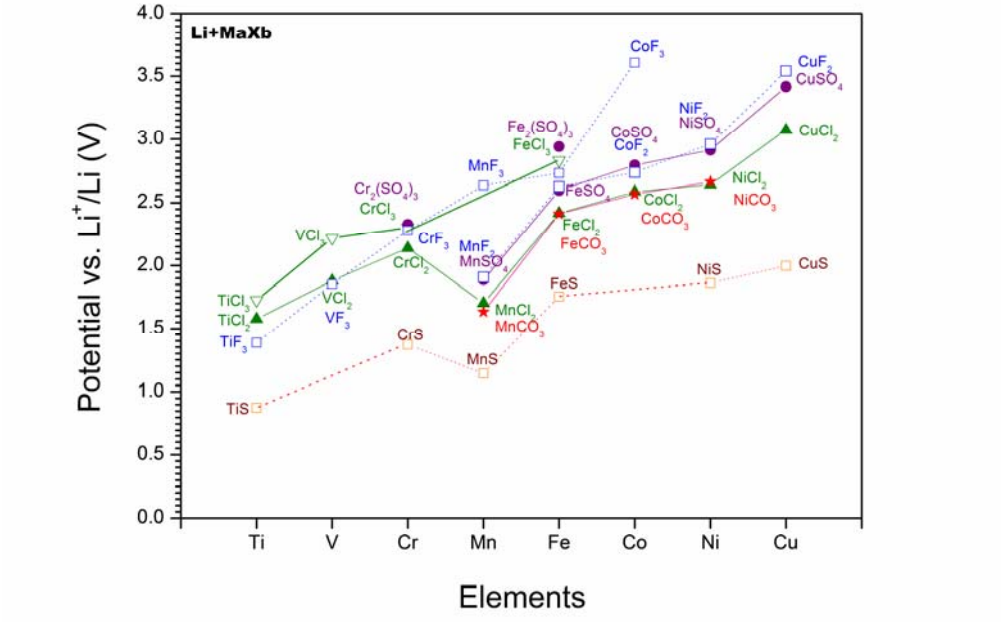


Figure S5. Calculated EMF values (V) of conversion reactions between binary transition mental compounds and sodium.

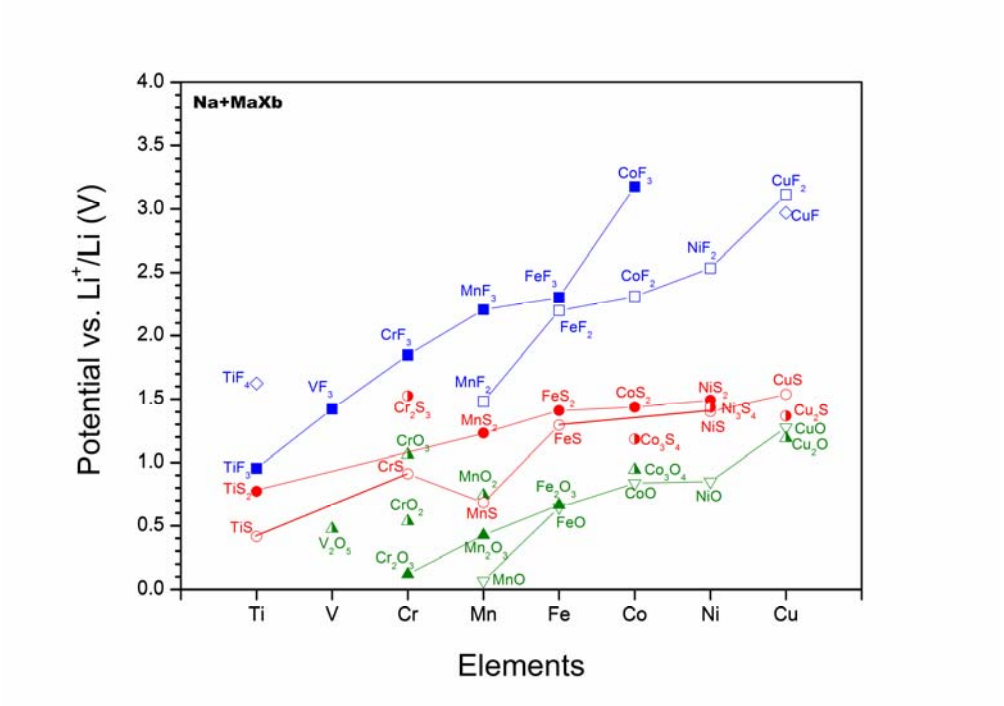


Figure S6. Calculated EMF values (V) of conversion reactions between binary transition mental compounds and magnesium.

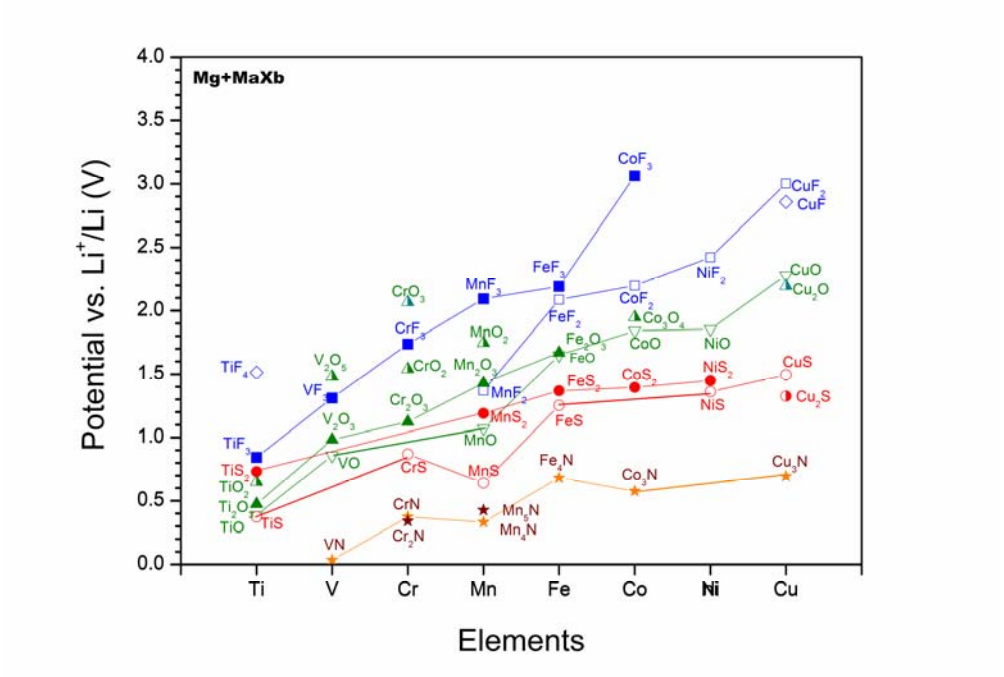


Figure S7. Calculated EMF values (V) of conversion reactions between binary transition mental compounds and aluminum.

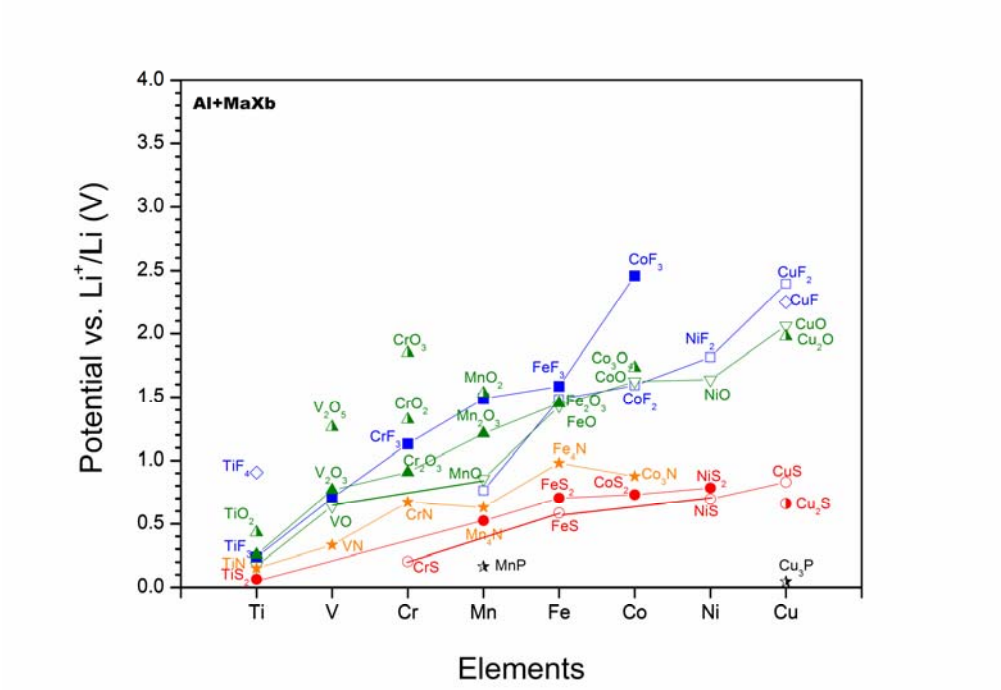


Figure S8. Calculated EMF (V) of conversion reactions between oxides and Li, Na, Mg or Al.

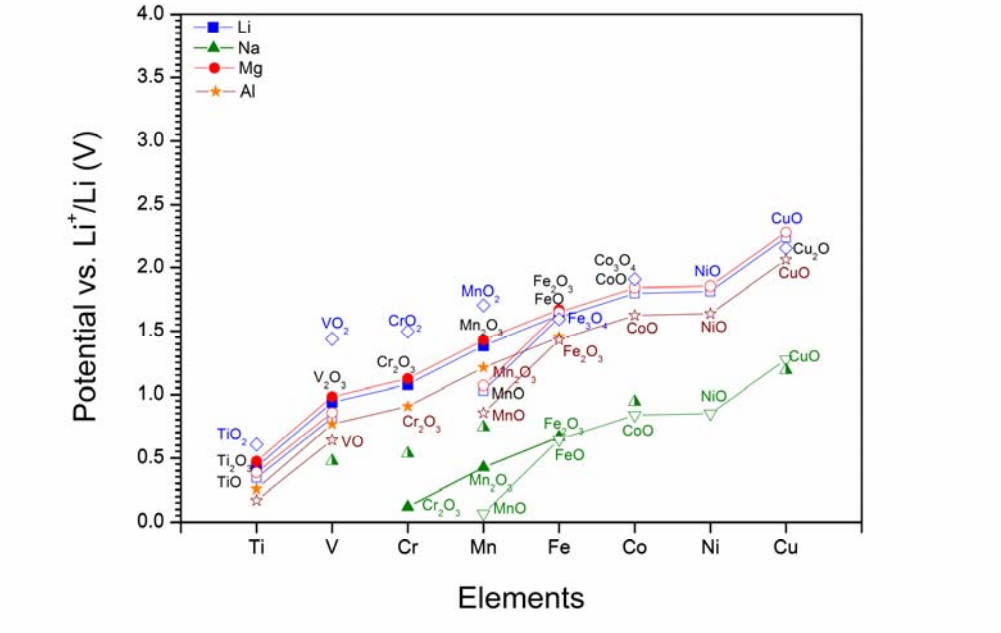


Figure S9. Calculated EMF (V) of conversion reactions between sulphides and Li, Na, Mg or Al.

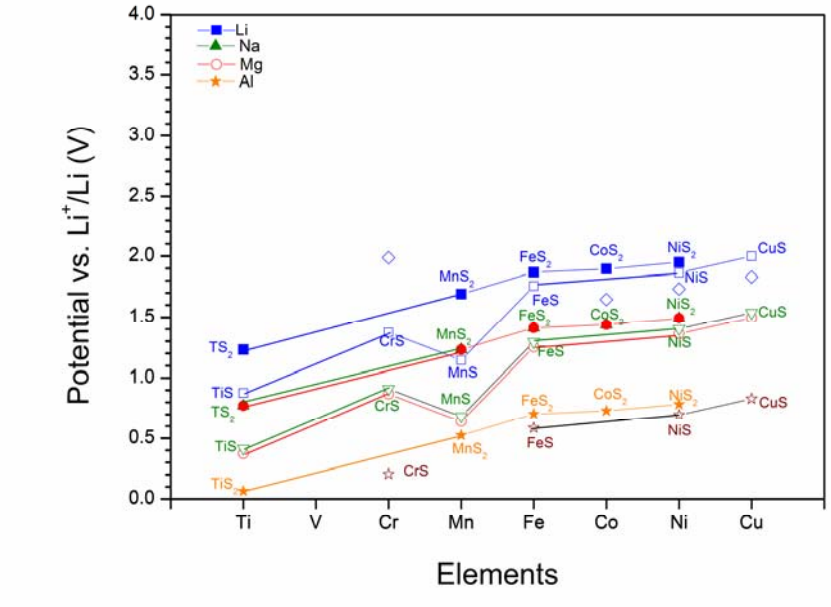


Figure S10. Calculated EMF (V) of conversion reactions between nitrides and Li, Na, Mg or Al.

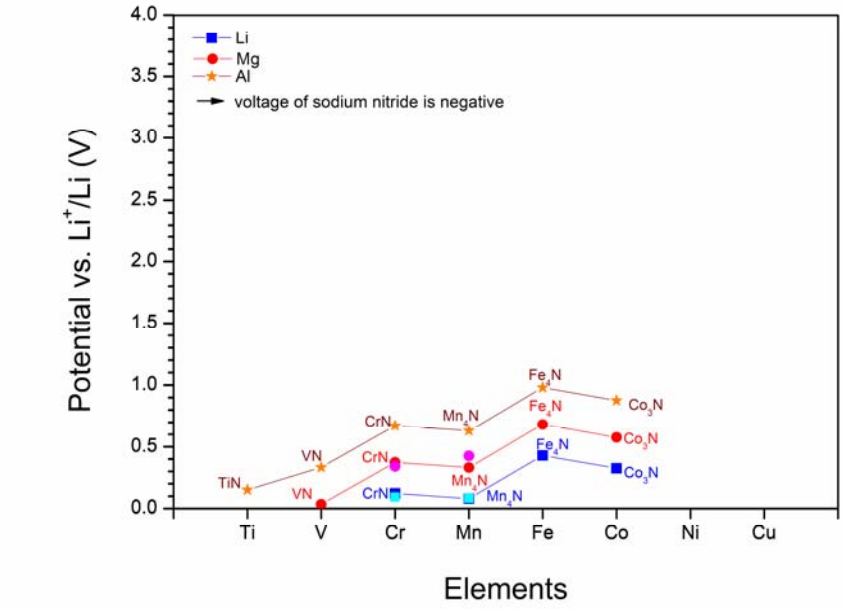


Figure S11. Calculated EMF (V) of conversion reactions between fluorides and Li, Na, Mg or Al.

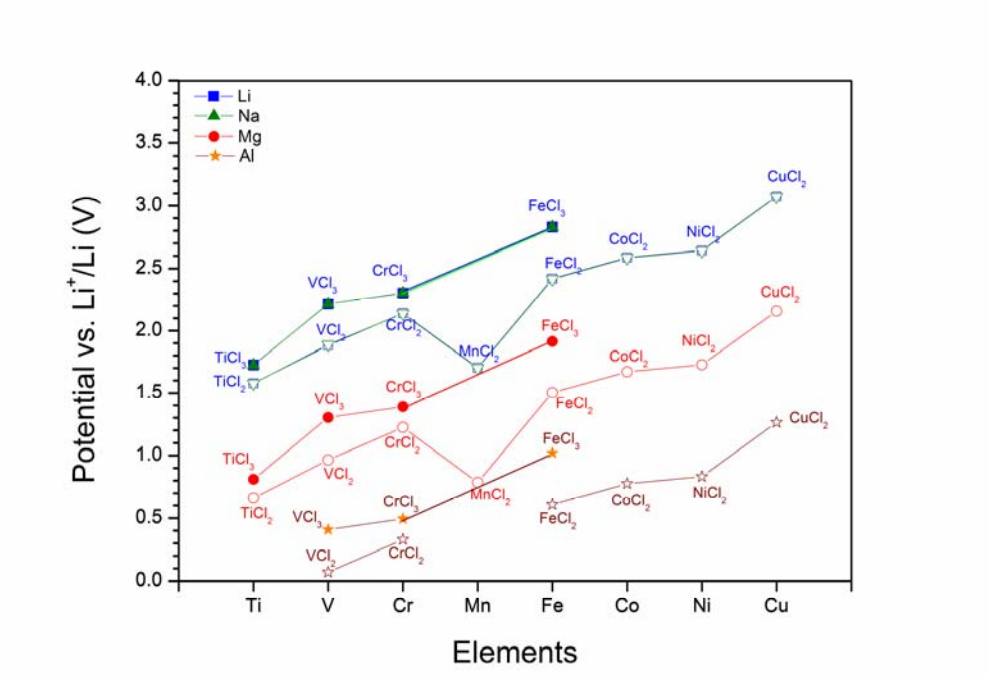
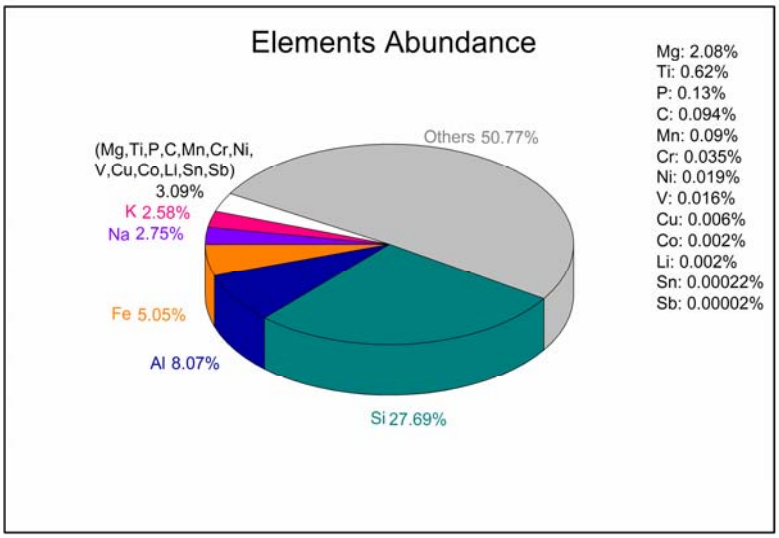


Figure S12. Elements abundance in the earth.



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