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Performance and resource considerations of Li-ion battery electrode materials

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In this work we present a data-driven approach to the rational design of battery materials based on both resource and performance considerations. A large database of Li-ion battery material has been created by abstracting information from over 200 publications. The database consists of over 16,000 data points from various classes of materials. In addition to reference information, key parameters and variables determining the performance of batteries were collected. This work also includes resource considerations such as crustal 10 abundance and the Herfindahl–Hirschman index, a commonly used measure of market concentration. The data is organized into a free web-based resource where battery researchers can employ a unique visualization method to plot database parameters against one another. This contribution is concerned with cathode and anode electrode materials. Cathode materials are mostly based on an intercalation mechanism, while anode materials are primarily based on conversion and alloying. Results indicate that cathode materials follow a common trend consistent with their crystal structure. On the other hand anode materials display similar behavior, based on elemental 15 composition. Of particular interest is that high energy cathodes are scarcer than high power materials and high performance anode materials are less available. More sustainable materials for both electrodes based on alternative compositions are identified.

Introduction

Depletion of non-renewable fossil fuels and environmental 20 pollution has driven researchers to seek alternative energy sources. The intermittent nature of green energy sources, such as hydroelectric, thermal, wind, and solar energy, illustrates the crucial role of efficient and cost-effective energy storage. One of the promising energy storage devices is the Li-ion battery, which 25 were developed in the 1970s, after the intercalation capability of dichalcogenides was discovered. Since their development, much research has been conducted to develop new materials and to improve battery performance and life. However, the complex nature of battery materials has made it difficult to identify robust 30 strategies for developing novel materials.

Influenced by the growing body of research, many studies reviewed important advances and breakthrough in the performance improvement of Li-ion batteries,[1-8] but only a few studies focused on battery cost and resource consideration. Jeong 35 et al [9] identified general issues for Li-ion batteries and emphasized the critical need for cheaper materials to meet high power electronics and transportation requirements. Argonne National Laboratory published a report concerning factors contributing to the cost of Li-ion batteries. They too concluded 40 that a significant contribution of cost is associated with materials by comparing the historical price of fundamental elements including cobalt, nickel, manganese and lithium.[10] Burke and Miller compared three materials for Li-ion batteries in electric vehicles (EVs) considering performance and cost.[11] In spite of 45 these and other reviews, the field lacks evaluation criteria with which to compare the performance and resource considerations of a variety of materials, both quantitatively and comprehensively.

One possible solution that has been successful in other fields is to explore correlation in large data sets. Prerequisite to a data-driven 50 approach is the development of quantifiable physical, chemical, and economic metrics that can be applied to data that is mined from the extensive Li-ion battery literature. The recent datamining study conducted by Gaultois et al. in the area of thermoelectric materials has demonstrated the advantages of such an approach.[12] 55 A key feature in the work by Gaultois et al. is the application of new visualization methods with high information density plots to facilitate the comparison and analysis of large data sets.

Given the large volume of information in the field, knowing the right data to extract is the first important step in the 60 datamining process. A battery is a device that converts chemical energy into electrical energy and vice versa. It consists of a cathode, which donates lithium in secondary batteries, an anode, the lithium acceptor, and an electrolyte that provides selective ionic transport while prohibiting electrical transport.[13] In this 65 study, the datamining process has been carried out for cathode and anode materials. The reason that we are concerned with just cathode and anode materials is that they contribute up to 30% of total cost of a battery cell. Additionally, they are also the primary parts in determining battery performance.[10] We have chosen 70 performance parameters to outline battery performance and application-limiting properties of batteries such as specific energy and specific power. Furthermore, to aid in future material discovery as well as to draw meaningful correlations between a material's performance and properties, we collected properties of 75 the material such as the structure type and synthesis route of the tested material along with reference data about the author and publication.

Enhancing the performance of a battery material is not the only challenge that needs to be overcome to make a compound

commercially viable. Economic factors such as cost, abundance, geopolitical activity, and market concentrations can significantly influence financial viability of a material. For example, for iron and manganese based cathode materials, the lithium availability is the principal resource concern. For cobalt and nickel based electrodes, the cost of electrodes is problematic.[10] Scarcity, the inverse of the weighted crustal abundance, and the Herfindahl−Hirschman Index (HHI) were used by Gaultois et al [12] to examine the economics of thermoelectric materials as they relate to geological abundance and market concentrations, respectively. The HHI indices, based on reserves and production, allow for uncoupled supply and demand analysis by quantifying the amount of known reserves as well as production for a given element as a function of geographical region.[14, 15] In this work we demonstrate how these economic indices for battery materials can be visualized simultaneously with performance parameters in order to aid the efforts of researchers to develop sustainable, high-performance, low-cost battery materials.

Methods

Nature and Source of Data

Data was abstracted from a large pool of literature on Li-ion batteries. The collected data represents experiments at both room temperature and at elevated temperatures (50-60°C). Most experiments have been carried out galvanostatically using a lithium anode with an organic electrolyte comprised of $LiPF_6$ solution in a composition of organic compounds such as ethylene carbonate, dimethyl carbonate, diethyl carbonate, or propylene carbonate. The data presented in Table 1 summarizes materials by primary elemental composition and associated publications used for this data driven review.

Table 1. General composition types of material and Publications from Which Data Was Extracted

Composition	References
Ni or Mn	16-69
Fe	55, 58, 70-93
Co	16, 30, 44, 58, 94-112
Cu	113-118
Si	25, 103, 119-128
Ti & Cr	129
Sb or P	27, 130-132
Sn	26, 104, 130, 133-140
V	141-146
Mo, C, Ge	103, 147-150

At the present time, there are nearly 16,000 database entries consisting of 26 categories associated with temperature of operation, electrode composition, mode of discharge, material family, electrolyte, reference electrode, structure, particle size, voltage of reaction, synthesis route, voltage window, discharge current, theoretical capacity, discharge capacity as a function of cycle (1st, 25th, 50th, 100th cycle), capacity loss per cycle, coulombic efficiency, rating performance, author, year of publication, DOI link, and comments. The lithium storage mechanism is another important parameter to consider. It was found that most of the electrodes operate based on an intercalation mechanism in which lithium ions are inserted or extracted from a material with an open crystal structure without major structural changes. On the other hand, some electrodes rely on a conversion mechanism that causes a structural change in the electrode through a reversible electrochemical reaction between lithium and an anion. This conversion mechanism has gained increasing attention recently and mostly occurs at a lower potential, appropriate for the role of the negative electrode. Lastly, alloying metallic or semi-metallic elements with lithium, is another reaction mechanism in electrode materials that works similarly to conversion. The development of the two latter mechanisms has been hindered by their poor life cycle that comes from large volume expansion and large voltage hysteresis.

Data from published work was extracted manually using free software, such as DataThief[151]. Cycling performance was reported in all papers while rating performance, cyclic voltammetry and differential capacity were reported in almost half of the published research data. Additional insight was obtained by using the extracted data to calculate rating performance, a measure of capacity retention at different current rates (C rates), which was used to compare battery materials at different C rates. Usually rating performance is reported through voltage capacity profile at different C rates. We adopted Shaju et al.'s definition[49] of rate capability for comparison purposes. The rate capability is expressed as the capacity at a given discharge rate relative to that obtained at a lower rate. We chose the ratio of discharge capacity at the discharge currents of 0.1 C, 1 C and 10 C. Extrapolation of the data at these discharge currents was generally avoided because the materials exhibited unexpected capacities at different discharge rates, specifically at higher discharge rates. The one case where data was extrapolated was when the capacity associated with 0.2 C discharge current was reported rather than the 0.1 C, since all materials exhibit a linear behavior in low discharge current.

Another challenge was reporting battery potential. Some researchers reported cyclic voltammetry and differential capacity data with which we determined average lithiation and delithiation potentials, but a single voltage value was required to calculate the approximate specific energy and power. For this we borrowed Bard and Faulkner's definition of mid-point potential to use for performance calculations.[152] We gathered this value for all references that reported voltage profile. Interestingly, the average potential was by a good approximation equal to the mid-point potential. Thus for those reports that had either plot, we accepted the value as an average potential.

Additional economic indices were generated directly from the anode/cathode chemical formula. HHI values for reserve and production were calculated from 2011 USGS commodity statistics using following formula $\sum_i^N S_i^2$ where N is the total number of countries consisted, and S_i is the percent market share of each country, i, in the world production or reserves of a given element. The U.S. Department of Justice and the Federal Trade Commission associated HHI < 1500 as an unconcentrated market, 1500 < HHI < 2500 as moderately concentrated, and HHI > 2500 as highly concentrated. Weighted HHI values were calculated using weight fraction of each element in the chemical formula. Elemental scarcity, which is crustal abundance in inverse parts per

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Table 2. Example parameter combinations for useful cathode material visualization schemes.

Abscissa	Ordinate	Size	Use	Finding
Average potential	Discharge capacity	Capacity retention	Performance and stability, Improvement domain, best material	Layered high capacity material, spinels and olivines high voltage
Specific power	Specific energy	any	Performance (Ragone plot)	High power Spinels~olivines v.s high energy layered
Capacity	Rating performance	any	High rate capability or rating performance	Spinels>olivines>layered
$HHI_{(production)}$	$HHI_{(reserves)}$	Specific power	Choice of material	Spinel best
$HHI_{(production)}$	$HHI_{(reserves)}$	Specific energy	Choice of material	Layered best
$HHI_{(production)}$	Scarcity	Capacity retention	Choice of material	Negative impact of precious metal additions

million (ppm), were calculated using elemental crustal abundance from the CRC Handbook.[153] Similarly to the HHI values, scarcity
5 was calculated based on the weight fraction of elements in the chemical formula. The formula $\zeta = \sum_i^N (\zeta_i \times (\frac{m_i}{m_{tot}}))$ was used to calculate scarcity, where ζ_i and m_i are the scarcity and weight of an element i in a material with N different elements.

Mechanics of Visualization

10 The datamining process included data extraction, database formation, and process visualization. Employing an appropriate visualization method is essential to interpret trends and correlations in such large data sets. The method of visualization used by Gaultois et al.[13] was adopted because it effectively
15 communicated relationships between many parameters. The website http://tomcat.eng.utah.edu/sparks/battery.jsp was developed to facilitate the organization and visualization of datamining results. In spite of having several parameters collected and tabulated, this website enables visualizing any combination
20 along the abscissa and ordinate. Also, this visualization introduces third and fourth dimensions by using variable marker size, the radius of a data point, and marker color to increase the information density that can be visualized in every plot. The user can sort material based on structure, material type, reaction
25 mechanism, temperature, and C rate. Hovering over a data point reveals a tooltip of information containing the chemical formula, temperature, synthesis route, voltage window, C rate, abscissa, ordinate, and marker values. Additionally, clicking on a data point will take the user to its reference.
30 In the following sections we will demonstrate the proficiency of this visualization method in the investigation and comparison of battery cathode and anode electrode materials by considering both performance and resource parameters.

Results and Discussion

35 In order to know what parameters are useful to plot, key parameters needed to be identified. For cathode materials, as indicated by Whittingham[154], the best materials are those with high capacity and high voltage that leads to high energy storage. Also, rapid reaction with lithium results in high specific power
40 and good rating performance, while high stability materials have

good cycling performance and high columbic efficiency.

Regarding anode materials, although the full-cell battery capacity is governed by the capacity of cathode material, a high capacity loading of an anode remains important. This importance
45 stems from the fact that a high capacity loading decreases weight, volume, and cost of the current collector and separator that eventually leads to a high energy storage material. Also, a lower anode voltage in a half-cell battery is favorable, since it increases a full-cell battery potential which is desirable for providing high
50 energy and high specific power. Nitta and Yushin indicated that potentials vs Li/Li$^+$ that are very close to zero increase dendritic formation that can lead to shorting the battery, while a potential higher than 0.8-1 V vs Li/Li$^+$ can prevent the formation of a solid electrolyte interface (SEI) which results in a more stable
55 material[7].

In this section we will examine general trends of electrode materials based on their reaction mechanism, structural type and elemental composition. While cathode and anode materials can be examined together, in this report we will consider them
60 separately for clarity. Each performance section will be followed by a discussion of resource considerations and then a simultaneous analysis of performance and resource parameters.

Cathode Performance Considerations

Many different plots can be generated and we encourage readers
65 to explore them via the free web-based resource. However, we list a few illustrative examples in Table 2 along with key findings for cathode materials. These plots will each be discussed in turn.

In Figure 1 we plot the average potential as a function of capacity with rating performance assigned to marker size and
70 structure type as marker color. The plot suggests that materials follow a common trend based on structure type; layered structures tend to have higher first discharge capacity, while materials with olivine and spinel structures display higher voltages. This plot includes all cathode materials, even those measured at different C
75 rates. Nevertheless, sorting data by C rate can confirm that this result is generally applicable. Olivine LiCoPO$_4$ [110] possesses the highest voltage and layered Li$_2$MnO$_3$-LiNi$_{0.44}$Co$_{0.25}$Mn$_{0.31}$O$_2$ [45] the highest capacity. As evidenced by the plot, no strong correlation is observed between the marker size and abscissa, ordinate or
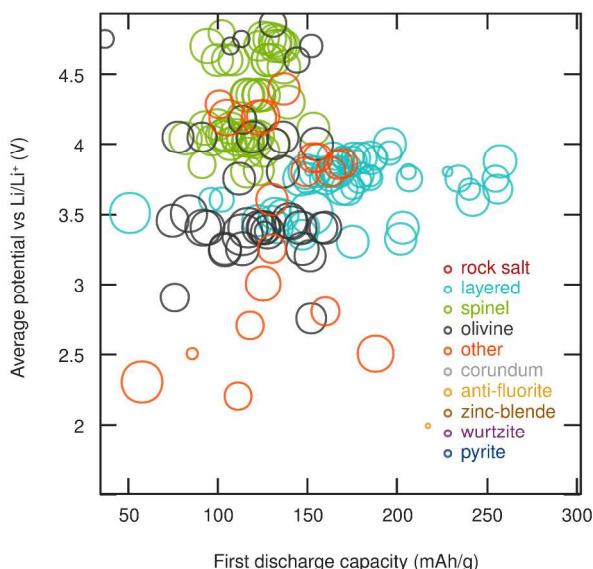
Figure 1. Average potential of a wide variety of cathode materials grouped by structural type is plotted against first discharge capacity. The marker size (radius) here is proportional to the capacity retention after 50th cycle.

5 structure type. High capacity retention and stability has been achieved by almost all intercalation materials at least up to the 50th cycle. Nevertheless, we can see that highest capacity retention corresponds to $Li_{1.375}Ni_{0.25}Mn_{0.75}O_{2.4375}$ [64] and $LiFePO_4$.[82] Moreover, $LiFePO_4$ [76-78, 81, 82, 89, 93] shows good

10 capacity retention at different C rates. About one third of collected papers reported cycling performance up to or beyond the 100th cycle. The best example of a high C rate capacity retention after 100th cycle belongs to $LiFePO_4$ [76] at 20°C and nano-$LiMn_2O_4$ [49] and $LiNi_{0.5}Mn_{1.5}O_4$ [48] at 10 °C.

15 One of the most typical plots for battery materials is a Ragone plot.[155] This plot visualizes the energy and power trade-off which allows performance comparison for different materials. The vertical axis describes available energy, while the horizontal axis shows the power that can be delivered and the sloping line

20 indicates the discharge rate corresponding to the power and energy values. A Ragone plot of cathode materials categorized by structure type, shown on the left of Figure 2, illustrates that

materials with layered structure possess the highest specific energy (996 Wh/kg for Li_2MnO_3-$LiNi_{0.44}Co_{0.25}Mn_{0.31}O_2$ at 0.09 C

25 [45]), whereas olivines and spinels have the highest specific power ($FePO_4$ [89] and $LiNi_{0.5}Mn_{1.5}O_4$ [48] with 11,050 W/kg and 6,900 W/kg respectively). Typically cobaltate materials are considered to be the best high specific energy materials,[156] but this demonstrates that non-cobalate layered materials, such as

30 $LiNi_{0.33}Li_{0.11}Mn_{0.56}O_2$,[44] can also have a very high specific energy. Furthermore, it can be seen that both the average potential versus first discharge capacity and specific power versus specific energy plots exhibit similar trends, except that olivines are serious competitors for spinels in specific power. It must be noted that

35 olivines have lower average potential than spinels, thus explaining the fast intercalation of lithium in olivine structure that provides high current while being stable. Nevertheless, when it comes to rating performance, spinels are still the best. Rating performance is defined as the capacity at a specified discharge rate relative to

40 that obtained at a lower discharge rate, where we chose discharge capacity at 1 C to that of 0.1 C for low rate capability and discharge capacity at 10 C to that of 1 C for high rate capability.

Plotting the rating performance as a function of first discharge capacity (Supporting Information) demonstrates the superior

45 rating performance of spinels over layered and olivine structures. The same result is observed at high rate performance and is consistent with the high power capability of spinels. Lithium has an octahedral coordination in common layered ($LiCoO_2$) and olivine ($LiFePO_4$) structures, whereas in the common spinel

50 ($LiMn_2O_4$) structure, it has a tetrahedral coordination.[156] This can explain fast lithium insertion in spinel structure which stems from more open sites. On the other hand, a 1D channel path in olivine structure can provide a fast diffusion path for lithium if the channel is not blocked.[4] Recent advancements in the heat

55 treatment and carbon coating of olivine materials have created unblocked paths that provide fast intercalation. The high specific energy of layered materials could also be attributable to the existence of multiple transition metal layers per unit cell.

It is worth noting that although factors such as particle and

60 pore size, electrode design and electrode composition can effect power, energy, and rate capability of material. These
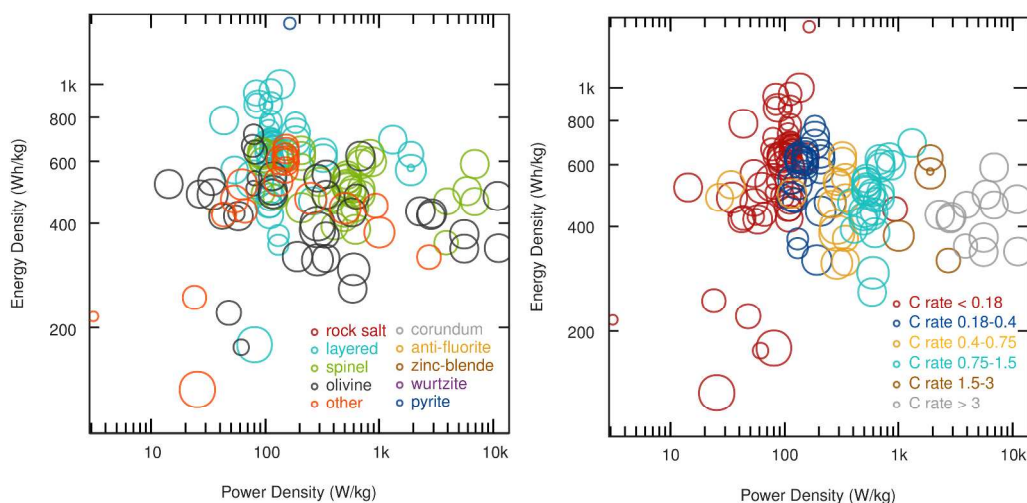

Figure 2. Ragone plot for a wide variety of cathode materials grouped by structural type (left) and C rate (right). The marker size is proportional to the capacity retention after 50th cycle in both plots.

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results indicate that the main parameter governing performance characteristics is crystal structure. Considering the relatively large amount of data it is unlikely that all of them have been designed to produce high rate capabilities.

5   By definition, coulombic efficiency is the ratio of the discharged capacity to the capacity needed to be charged to the initial state before discharge.[157] Inefficiency comes from a side reactions such as material corrosion and electrolyte decomposition, etc. Plotting the coulombic efficiency versus the 10 average potential (Supporting Information) shows a lower coulombic efficiency of layered structures that can be attributable to slow diffusion of lithium and population at the surface of the layered material.[158] Lower coulombic efficiency at higher potentials is also expected;[5] however, spinels exhibit a highly 15 stable performance.

Cathode Resource Considerations

The parameters beyond performance will be reviewed and discussed in this section. There are numerous resource considerations that can limit material applications, including 20 toxicity, abundance, recyclability, availability, cost, chemical compatibility, and many others. A combined analysis of performance and resource considerations is critical to determine how promising a material is for widespread application. In this report, we use an elemental composition of materials to calculate 25 the scarcity, which is based on crustal abundance, and the Herfindahl-Hirschman Index (HHI), an economic measure for estimating the availability and supply risk of materials based on known reserves as well as production. The development of these economic indices was discussed in the methods section. Analysis 30 of cost, toxicity, and recyclability are not included because general quantitative measurements of these parameters have not yet been established.

Plotting scarcity against HHI_P for cathodes (Figure 3) is useful to identify the potential costs and resource barriers for high

35 performance materials. Encoding specific energy as marker size illustrates that high-performance layered materials are a factor of 2 to 4 times more scarce than olivines and spinels, though they are capable of achieving twice the specific energy. Therefore, there is a trade-off between the specific energy and the scarcity that must 40 be considered in the choice of cathode material. In the case of layered cobaltate materials, the HHI_P factor is approaching 2500, which is the limit set by the United States Department of Justice and Federal Trade Commission for highly concentrated, monopolistic production of a commodity. Incorporation of cobalt 45 in cathode material increases HHI_P by a factor of two without significant increase in performance of material.

Cobaltates are the primary material in many commercial lithium ion batteries. Their advantages consist of high discharge capacity, ease of production, stable cycling and oxygen loss 50 reduction which improved safety,[156] but the high cost of cobalt always has been a concern and motivation for finding new materials. In addition, when considering capacity retention upon cycling, cobaltate materials do not have better stability than other materials. These findings reinforce the potential to reduce battery 55 costs by replacing cobalt with less expensive and more widely available alternative materials.

By switching the marker size to specific power and keeping the same axes, the plots now show that olivines and spinels have a high specific power and are more abundant compared to layered 60 materials. The HHI_P factor for olivines and spinels varies greatly and depends on whether iron or manganese is the integrated material.

The only conversion-based cathode material, the pyrite FeS_2, cannot compete with other materials in power, but has two times 65 as much energy as layered materials, and is 7 times more abundant. This shows that this conversion-based cathode material can be a serious candidate for future energy storage applications if cycling stability issues can be overcome.
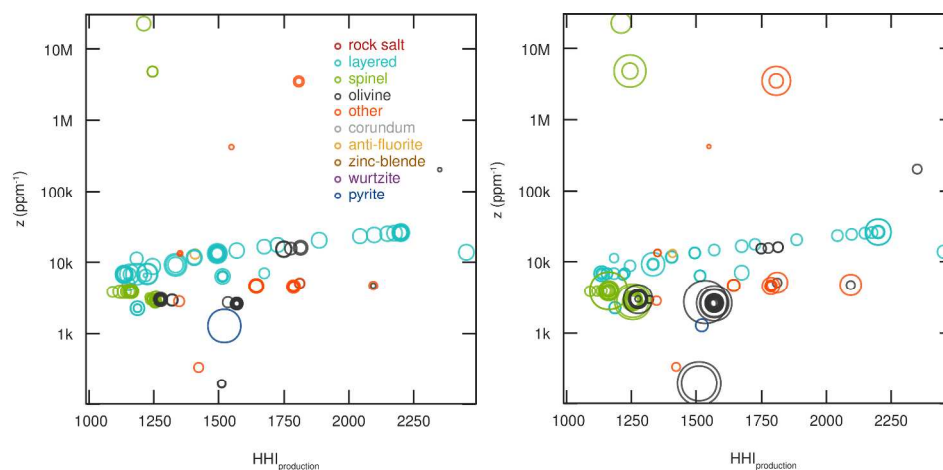
70   Figure 3. A resource considerations plot, showing scarcity vs. HHI_P of a wide variety of cathode materials grouped by structural type. The marker size is proportional to specific energy (left) and specific power (right).

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Table 3. Example parameter combinations for useful Anode material visualization schemes.

Abscissa	Ordinate	Size	Use	Finding
Average potential	First discharge capacity	Capacity retention	Best material	Silicon based materials are good candidates for next generation anodes
Average potential	First discharge capacity	Coulombic efficiency	Effect of potential on SEI formation	SEI formation may not be a factor of potential
HHI_P	Scarcity	Capacity retention, first discharge capacity, average potential	Analysis of factors relating to cost.	High scarcity of antimonate

Anode Performance Considerations

5 Carbonaceous materials have long been the standard for battery anode materials. Recently, alloy and conversion-based materials have shown a high potential for replacing the conventional carbonaceous materials since they have a significantly higher loading capacity, resulting in batteries with high power and 10 specific energy. Table 3 identifies a few informative plots for visualizing the datamining results of anode materials.

Visualizing the first discharge capacity as a function of average potential and employing capacity retention as a marker size provides fundamental information about different lithium reaction 15 mechanisms by sorting material based on this factor. Alloy-based materials lie in the high capacity and low potential region while conversion-based materials exhibit higher potentials and are less stable upon cycling. The biggest challenge that alloy and conversion anode materials face is their poor cycling 20 performance.   In the left plot of Figure 4 we can compare materials based on their performance and stability.

In contrast to cathode materials, alloy based anodes do not follow a common trend based on crystal structure, but rather, they exhibit trends based on elemental composition. As described in 25 the methods section, the best anode materials have a low voltage, high capacity, and high capacity retention. Under this definition, SiC [126] would appear to be the best material and is found at the upper left corner of the graph with decent capacity retention. Tin- and silicon-based materials have a low average potential. These 30 materials along with alloy anodes based on phosphorus and antimony, and conversion based cobaltates tend to have a high capacity retention upon cycling compared to others. On the other hand, alloy-based silicon, germanium, and conversion based ZnO[149] and VN[141] compounds tend to have a higher capacity. 35 Taken together, silicon based material are good candidates for next generation of anode materials.

Normally it is thought that high voltage means less SEI[7] layer formation and one would expect better capacity retention and higher coulombic efficiency upon cycling. However, by switching 40 marker size to columbic efficiency as shown in the image on the right of Figure 4, one can see that there is a high columbic efficiency at a lower potential. Since columbic efficiency can be
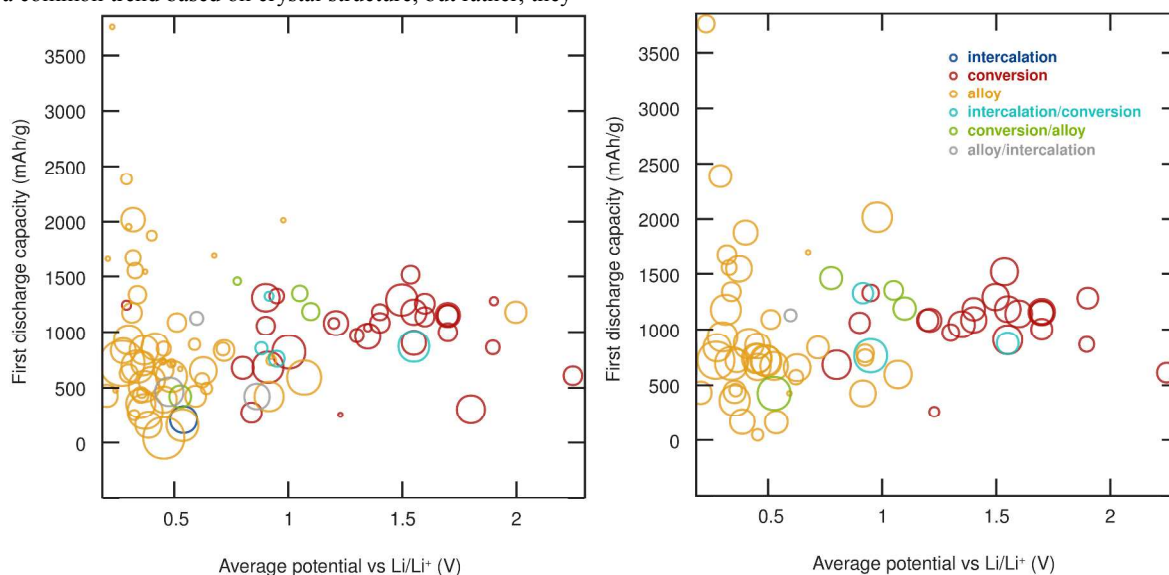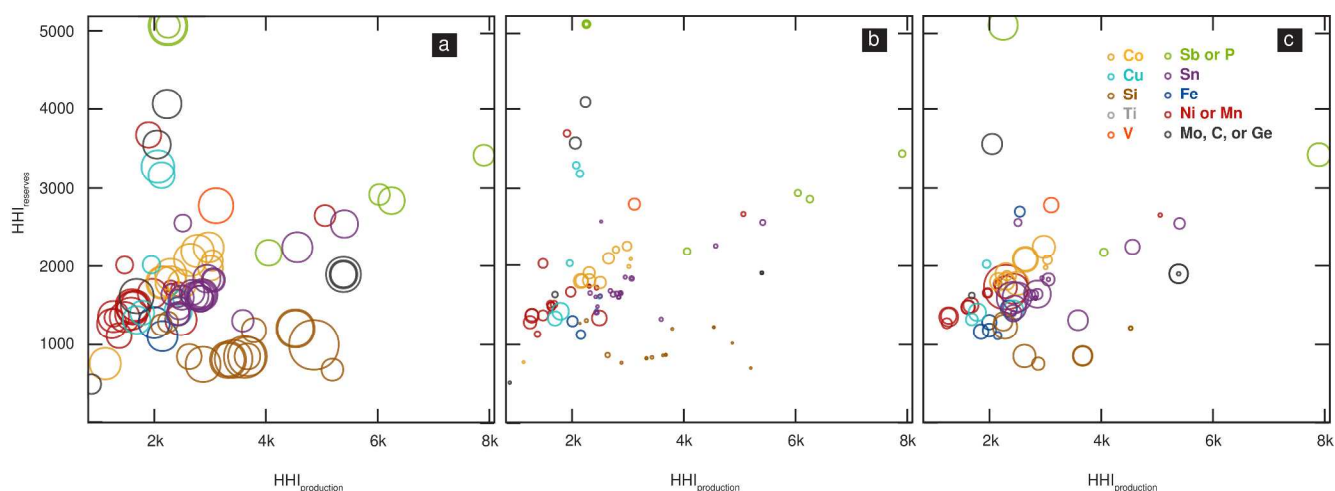

45 Figure 4. First discharge capacity of a wide variety of anode materials grouped by Li storage mechanism s plotted against average potential. The marker size is proportional to the capacity retention after 25th cycle (left) and coulombic efficiency (right).

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5 Figure 5. Resource consideration of a wide variety of anode materials grouped by material composition, HHIR is plotted against HHIP. The marker size is proportional to (a) first discharge capacity, (b) average potential, and (c) capacity retention at 50th cycle.

considered as a measure of SEI layer formation[157]. It must be noted that other factors such as volume change and voltage hysteresis are also responsible for lowering coulombic efficiency 10 and capacity retention upon cycling. Considering Figure 4 which provides coulombic efficiency and capacity retention of first cycle, we can conclude that the aforementioned idea about anode materials is not necessarily true.

Another combination of parameters that yields valuable 15 meaning is plotting the average potential against the voltage hysteresis (Supporting Information). Large voltage hysteresis between charge and discharge results in a poor energy efficiency. The voltage hysteresis values increase with increasing potential. Furthermore it shows that high voltage hysteresis is mainly 20 associated with conversion-based materials, featuring the fact that higher energy materials have a lower energy efficiency.

Anode Resource Considerations

As with cathode materials, plotting resource considerations as 25 abscissa and ordinate parameters, including HHI$_P$, HHI$_R$, and scarcity; simultaneously with performance factors, such as capacity, voltage or capacity retention; as marker size offers insight into the commercial viability of high performance materials based on cost and availability. Assigning first discharge 30 capacity to the marker size, as seen in Figure 5a, reveals that materials based on Mn, Ni, Cu, and Zn have the lowest market concentration and a relatively high capacity around 1500 mAh/g. Although this capacity is lower than the highest capacity material, SiC[126], HHI$_P$ is a factor three times lower. Also it must be noted 35 that HHI$_R$ for SiC is very low and the high HHI$_P$ can be attributed to USGS data for high quality semiconductor grade silicon. If low

purity silicon can be used for SiC then the HHI$_P$ would also be much lower. There are several studies concerning application of antimony-based compounds for anode material, but this material 40 has highest supply risk. For example, antimony[132] is located at the top right corner of the plot with highest availability and supply risk, and possess HHI$_P$ and HHI$_R$ factor of 16 and 6 respectively, relative to the C with the lowest resource risk.

With the average potential as marker size, see Figure 5b, the 45 lowest potential materials can be seen to have 2-4 times higher HHI factors compared to materials with higher potential. Furthermore, plotting the capacity retention as marker size, as in Figure 5c, shows that there is a minimum, but tolerable, market concentrations for achieving high cycling performance.

50 For wide-spread deployment of materials, incorporation of scarce elements becomes important. Plotting scarcity and HHI$_P$ with capacity retention as marker size, (see Supporting Information), it can be seen that tin-based materials possess better cycling performance. For example, Sn[133] has 100% capacity 55 retention after 50 cycle and is several orders of magnitude more scarce than SiC[126] with capacity retention of 67% after 50 cycles. With first discharge capacity as marker size, (Supporting Information), it can be seen that a high capacity is achievable even at low HHI factor and with abundant material. Finally, 60 considering the average potential as marker size, silicon-based materials offer a good combination of resource considerations and low average potential materials.

Conclusions

This paper provides an overview of the large domain of battery 65 materials, including cathode and anode electrode materials. The approach employed allows researchers to focus on property

regions, material families and structure types that are best suited for a given application. Simultaneous analysis of performance and resources has been provided using a multi-dimensional visualization method. Cathode materials have shown a similar property-based tendency, based on their structure type. This behavior can be described by virtue of their structure type. Spinels and olivines tend to show high power capability, while layered structures exhibit high energy capability. This shows that there is a potential to produce structural compositions to facilitate both high energy and power properties. Results show that spinels have a better rating performance over layered and olivine structures, which is consistent with the high power capability of spinels. The layered structure also possesses a lower columbic efficiency.

Resource consideration indicates that high performance layered materials are a factor of 2 to 4 times more scarce than olivines and spinels, though they are capable of achieving twice the specific energy. In other words, olivines and spinels have a high specific power and are more abundant materials compare to layered structures. Therefore there is a trade-off between specific energy and scarcity that must be considered in the choice of cathode materials. For anode materials, tin- and silicon-based materials have a low average potential and high capacity retention upon cycling when compared others. Increasing voltage hysteresis values with increase in potential indicates that high voltage hysteresis is mainly associated with conversion-based materials and the fact that higher energy materials have lower energy efficiency.

Resource considerations for anode material illustrates that the lowest potential materials have 2-4 times higher HHI factors compared to materials with a higher potential. Also there is a minimum, but tolerable, market concentrations for achieving a high cycling performance. It must be noted that achieving high performance is possible even with using abundant and low risk available material. As for cathode materials, abundant materials such as Si, Mn, Ni, Cu, and Zn have the potential to achieve high performance capability and there is no need for the use of precious materials, such as antimony.

Acknowledgements

Notes and references

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