Computational Screening of Future Cathode Materials Lithium-Ion Batteries

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Abstract

As the most common type of rechargeable battery, Lithium-ion batteries provide a safe and quick way to store and convert energy on a daily basis in phones and other electronic accessories. The most common commercial battery materials are layer-structured is $LiCoO_2$ which has been known to be used in Tesla and Apple products. The main issue presented by this battery material is the limited energy density, which hinders its application in a few key markets including the extended-range electric vehicles. Using a computational approach, this project screened potential cathode materials with improved energy density, and at least one promising alternative to replace $LiCoO_2$ has been identified. The economic and environmental impacts of this new material have also been analyzed. While additional studies are required to confirm the electrochemical stability of the material, our results could lead to a potential breakthrough in the next-generation high-energy density batteries.

Introduction

Current Industrial Lithium-ion batteries are limited in energy density, which causes a limited running time and use. Our research indicates that changing the cathode (negative terminal) material has a chance to increase the energy density of the battery. The voltage and capacity of the battery will change because the different cathode material will also change. Lithium-ion batteries used in cellphones and electric cars are essential in everyday life and the research towards these batteries will improve battery life by increasing the energy density.

Table 1. $LiCoO_2$ Electrochemical Characteristics

Material	Voltage [V]	C (capacity) [mAh/g]	Energy Density [Wh/kg]
$LiCoO_2$	3.9	190	840

Methods

MedeA was used as a GUI (Graphical User Interface) to preform VASP calculations. VASP is a software to preform quantum mechanical calculations. By running VASP, the structure of the material was optimized to find the lowest energy state of the compound. By finding the most stable form of the compound, the energy density calculations from VASP will be accurate.

Capacity Sample Calculations

Example: Li_3NiF_6

Reaction: $3Li + Li_3NiF_6 \rightarrow\ 6LiF + Ni$

$$C = \frac{3 * 1.6 \times 10^{-19}}{\frac{((3*6.941)+58.693+(6*18.998))}{6.02 \times 10^{23}}} \frac{Coulomb}{g}$$

$$C = 1493.302\, \frac{Coulomb}{g} \times \frac{1000}{3600}\, mA * h$$

$$C = 414.806\, \left(\frac{mA*h}{g}\right)$$

Multiplying factor (n): 3
Charge of Electron: 1.6×10^{-19}
Avogadro's Number: 6.02×10^{23}

Voltage Sample Calculations

Example: Li_3NiF_6

Reaction: $3Li + Li_3NiF_6 \rightarrow\ 6LiF + Ni$

$\Delta E = E(\text{products}) - E(\text{reactants})$
$\Delta E = E(Ni) + 6E(LiF) - E(Li_3NiF_6) - 3E(Li)$
$\Delta E = -11.592$ eV
$V = -\frac{\Delta E}{n} = -\frac{-11.592}{3} = 3.864$ V

Energy Density Sample Calculations

Example: Li_3NiF_6

Energy Density = Voltage * Capacity = 3.864 * 414.806
Energy Density = 1602.810 Wh/kg

Results

Table 2. Possible Cathode Materials

Material	Voltage [V]	C (capacity) [mAh/g]	Energy Density [Wh/kg]
Mn_2NiO_4 [2]	1.768	920.6697	1627.16
Na_3FeF_6 [3]	1.793	672.242	1205.33
$CuFeO_2$ [4]	1.803	706.935	1274.60
$AsCoLiO_4$ [5]	1.944	914.836	1778.441
$CsSbF_4$ [6]	2.04	323.66	660.27
Ag_2NiO_2 [7]	2.281	349.254	796.65
$NaAgF_4$ [8]	3.369	517.385	1743.07
Li_3NiF_6 [9]	3.864	414.806	1602.810

Cathode Material One: $AsCoLiO_4$

Reaction: $7Li + AsCoLiO_4 \rightarrow 4Li_2O + As + Co$

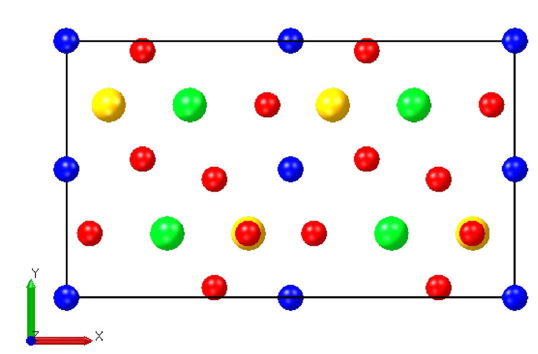

Figure 1. $AsCoLiO_4$ relative to X & Y axis[5]

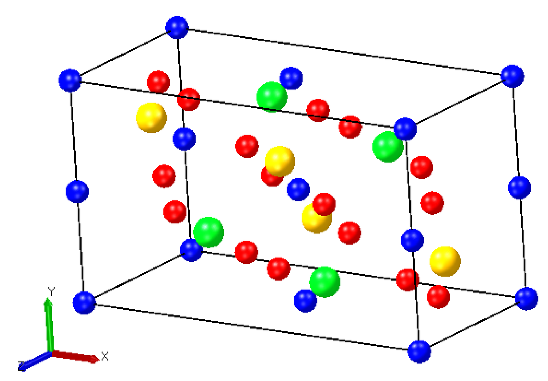

Figure 2. $AsCoLiO_4$ relative to X, Y, Z axis[5]

As: Arsenic | Yellow Dots
Co: Cobalt | Green Dots
Li: Lithium | Blue Dots
O: Oxygen | Red Dots

Cathode Material Two: $NaAgF_4$

Reaction: $4Li +\ NaAgF_4 \rightarrow 4LiF + Na + Ag$

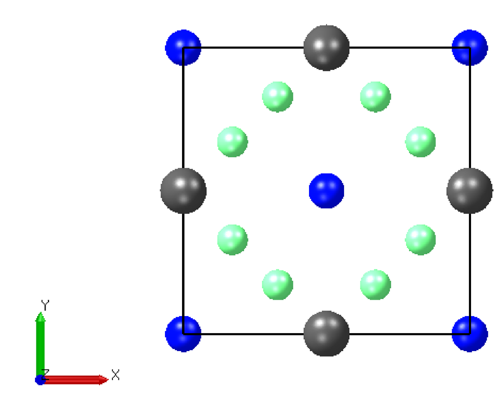

Figure 3. $NaAgF_4$ relative to X & Y axis[8]

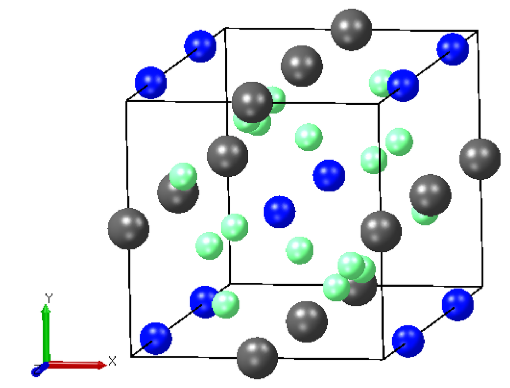

Figure 4. $NaAgF_4$ relative to X, Y, Z axis[8]

Na: Sodium | Dark Blue Dots
Ag: Silver | Grey Dots
F: Fluorine | Light Green Dots

Cathode Material Three: Mn_2NiO_4

Reaction: $8Li + Mn_2NiO_4 \rightarrow 4Li_2O + 2Mn + Ni$

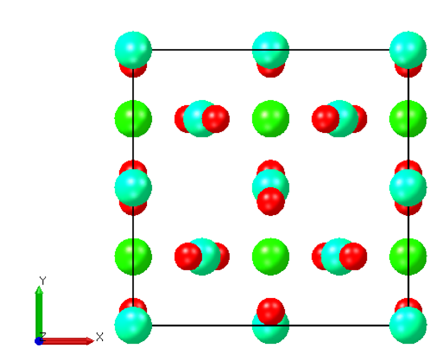

Figure 5. Mn_2NiO_4 relative to X & Y axis[2]

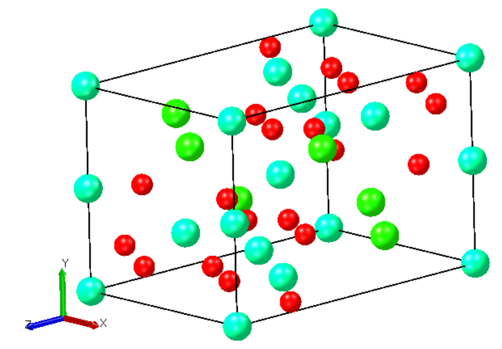

Figure 6. Mn_2NiO_4 relative to X, Y, Z axis[2]

Mn: Manganese | Light Green Dots
Ni: Nickel | Green Dots
O: Oxygen | Red Dots

Discussion

Table 3. Summary of optimum cathode Materials

Material	Voltage [V]	C (capacity) [mAh/g]	Energy Density [Wh/kg]
$AsCoLiO_4$	1.944	914.836	1778.441
$NaAgF_4$	3.369	517.385	1743.07
Mn_2NiO_4	1.768	920.6697	1627.16
$LiCoO_2$	3.9	190	840

$\underline{AsCoLiO_4}$: Cobalt has a dangerous environmental impact, high cost, and low availability; however, a high energy density and strength.
$\underline{NaAgF_4}$: Sodium is abundant and inexpensive, and Fluorine is also inexpensive. Fluorine is very reactive and could cause production issues if not handled correctly. Ag is relatively expensive and insufficient for large production.
$\underline{Mn_2NiO_4}$: Manganese is very abundant and inexpensive but is harmful to the environment if not contained properly. Nickel is environmentally destructive, but relatively expensive and great to work with industrially.

As seen in Table 3, $AsCoLiO_4$, $NaAgF_4$, and Li_3NiF_6 succeed in increasing the energy density compared to $LiCoO_2$**.** As promising alternatives, the electrochemical stability of these materials can be analyzed in future studies. Other factors such as the environmental impact, cost, etc. are essential in the consideration of producing next-generation industrial Lithium-ion batteries.

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