Computational Screening of Future Cathode Materials for Sodium-Ion Batteries

Matthew Glaus | University Transfer, Chippewa Valley Technical College

Dr. Ying Ma | Department of Materials Science and Biomedical Engineering, University of Wisconsin Eau Claire

Abstract

Sodium-ion batteries are the, often, overlooked relative of lithium-ion batteries. Lithium is a great anode material for batteries, but natural lithium supplies are dwindling. Sodium, on the other hand, may work as a replacement anode material. Using a computational approach this project screens potential cathode materials, for Na-ion batteries, with improved energy density to compete with overused Li-ion batteries. One potential cathode material for Na-ion batteries, that can compete with Li-ion batteries, has been identified. While additional studies are required to confirm the electrochemical stability of the material, these results could lead into future breakthroughs for Sodium-ion batteries.

Introduction

Right now, the commercial market is saturated with Li-ion batteries. Lithium may be a great material when used in a battery, but it's expensive and scarce. Na-ion batteries use the same working principles as Li-ion batteries. With some cathode materials, Na-ion batteries come close, and in some cases surpass, Li-ion batteries in energy density. Li-ion batteries currently being used in cellphones and electric vehicles are not very energy dense which causes a lower running time. This research indicates that, depending on the cathode material, Na-ion batteries have the potential to surpass Li-ion batteries in energy density.

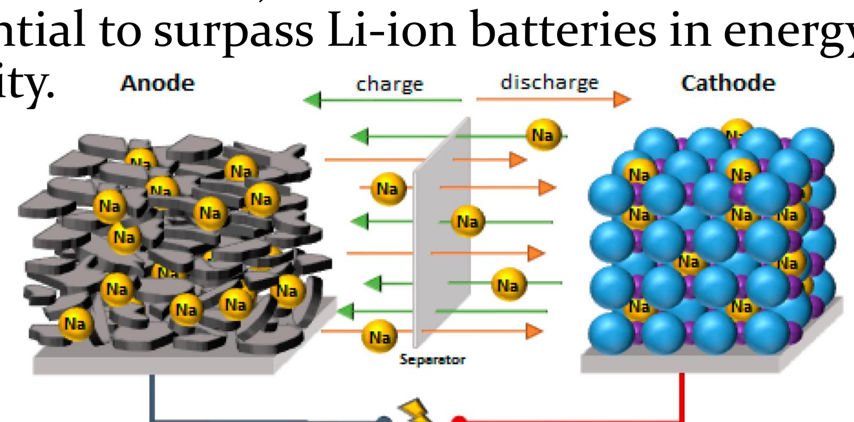

Figure 1. Working principle of a Sodium-ion cell[1]

Methods

The program MedeA was used as a GUI (Graphical User Interface) to find prospective cathode materials perform VASP calculations with them. VASP is a software that was used to perform quantum mechanical calculations. With VASP a material's structure was optimized to determine the material's lowest energy state. Through these calculations a compound's most stable form was found, which gave the most accurate VASP energy value (in eV), and the compound's energy density could then be calculated.

Capacity Sample Calculations

Example: $NaVO_2$

Reaction: $Na + VO_2 \leftrightarrow NaVO_2$

$$C = \frac{1 * 1.6\times10^{-19}}{\frac{50.942+(2*15.999)}{6.02\times10^{23}}} \frac{Coulomb}{g}$$

$$C = 1161.321 \frac{Coulomb}{g} \times \frac{1000}{3600} mA * h$$

$$C = 322.6 \left(\frac{mA * h}{g}\right)$$

Multiplying factor (n = # of Na atoms added to Cathode): 1

Charge of Electron: 1.6×10^{-19}

Avogadro's Number: 6.02×10^{23}

Voltage Sample Calculations

Example: $NaVO_2$

Reaction: $Na + VO_2 \leftrightarrow NaVO_2$

ΔE=E(products)–E(reactants)

$\Delta E = E(NaVO_2) - (E(VO_2) + E(Na))$

ΔE= -1.428 eV

$$V = -\frac{\Delta E}{n} = -\frac{-1.428}{1} = 1.4 \text{ V}$$

Energy Density Sample Calculations

Example: $NaVO_2$

Reaction: $Na + VO_2 \leftrightarrow NaVO_2$

Energy Density = Voltage * Capacity = 1.4 * 322.6

Energy Density = 451.6 Wh/kg

Results

Table 1. Structures of screened materials

Material	Space group	Lattice constant (Å)		
		a	b	c
$NaVO_2$[2]	R-3m	2.970	2.970	16.549
$NaCuO_2$[3]	C2/m	6.555	2.831	6.253
$NaCrO_2$[4]	R-3m	2.927	2.927	16.472

Cathode Material One: $NaVO_2$

Reaction: $Na + VO_2 \leftrightarrow NaVO_2$

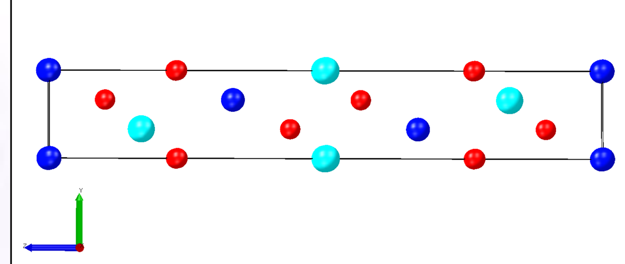

Figure 2. $NaVO_2$ relative to X & Y axis[2]

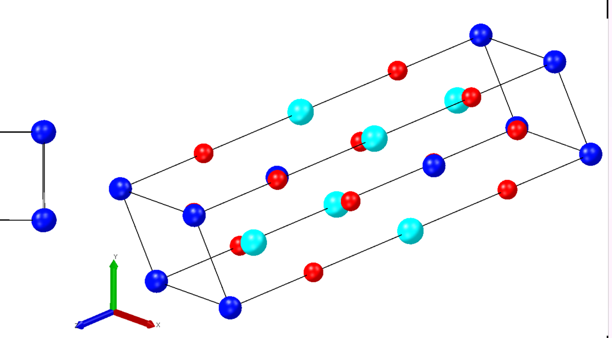

Figure 3. $NaVO_2$ relative to X, Y, & Z axis[2]

Na: Sodium | Blue Dots

V: Vanadium | Light Blue Dots

O: Oxygen | Red Dots

Cathode Material Two: $NaCuO_2$

Reaction: $Na + CuO_2 \leftrightarrow NaCuO_2$

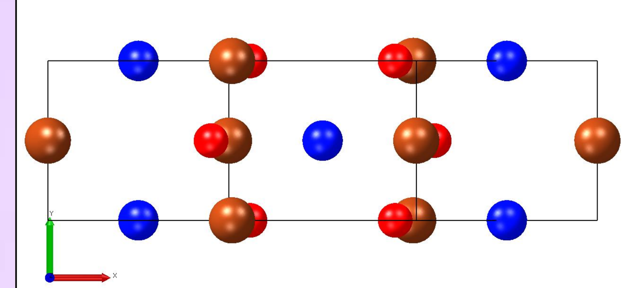

Figure 4. $NaCuO_2$ relative to X & Y axis[3]

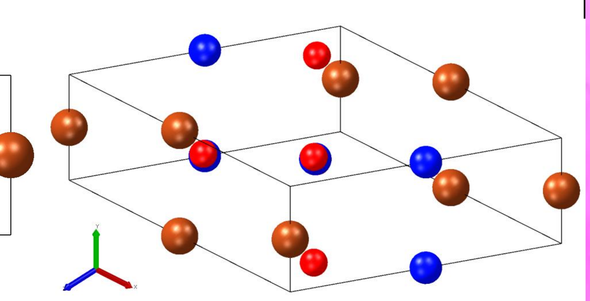

Figure 5. $NaCuO_2$ relative to X, Y, & Z axis[3]

Na: Sodium | Blue Dots

Cu: Copper | Brown Dots

O: Oxygen | Red Dots

Cathode Material Three: $NaCrO_2$

Reaction: $Na + CrO_2 \leftrightarrow NaCrO_2$

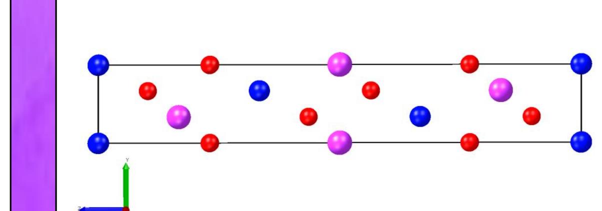

Figure 6. $NaCrO_2$ relative to X & Y axis[4]

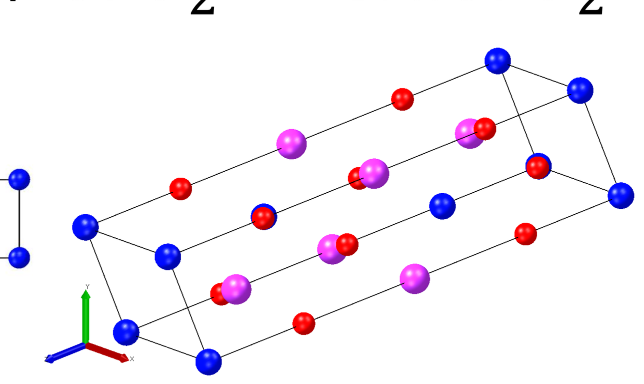

Figure 7. $NaCrO_2$ relative to X, Y, & Z axis[4]

Na: Sodium | Blue Dots

Cr: Chromium | Purple Dots

O: Oxygen | Red Dots

Discussion

Table 2. Summary of computed cathode materials

Material	Voltage [V]	C (capacity) [mAh/g]	Energy Density [Wh/kg]
$NaVO_2$	1.4	322.6	460.6
$NaCuO_2$	2.8	280.0	780.2
$NaCrO_2$	0.3	318.5	105.8
$LiCoO_2$	3.9	190	840

$\boldsymbol{NaVO_2}$: Vanadium is naturally abundant and is commonly obtained as a by-product from petroleum refining. However, obtaining large quantities of Vanadium is difficult. Vanadium is also very expensive. Sodium is abundant and inexpensive.

$\boldsymbol{NaCuO_2}$: Copper is a scarce resource and mining for copper has detrimental impacts on the environment. Copper is also used for many commercial products, so it is only becoming scarcer. Sodium is abundant and inexpensive.

$\boldsymbol{NaCrO_2}$: Chromium is naturally abundant and highly toxic. Mining for chromium is considered a serious threat to the environment and public health. Sodium is abundant and inexpensive.

Conclusion: As seen in Table 2 $NaVO_2$ has about half the energy density of the common Li-ion cathode material $LiCoO_2$. $NaCuO_2$, on the other hand, comes very close to the energy density of $LiCoO_2$. This is a promising start that gives us hope of finding better cathode materials. Although the electrochemical stability of the cathode materials still needs to be studied, at least computationally, sodium-ion batteries can compete with lithium-ion batteries.

References

[1] Daniel, C.; Besenhard, J.O. *Handbook of Battery Materials*; John Wiley & Sons: Weinheim, Germany, 2012. [Google Scholar]

[2] Chamberland B.L. and Porter S.K., *Journal of Solid State Chemistry*() 73, 398 – 404 (1988)

[3] Brese N.E., O'Keeffe M., Von Dreele R.B. and Young V.G. Jr., *Journal of Solid State Chemistry*() 83, 1 – 7 (1989)

[4] England W.A., Goodenough J.B. and Wiseman P.J., *Journal of Solid State Chemistry*() 49, 289 – 299 (1983)

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