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Powering the Future: Understanding Lithium-Ion Batteries

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Summary

- Background
- Introduction to lithium-ion batteries
- Challenges
- Solutions

Background

- **PhD studies (2016-2021):** I worked alongside Dr. Jeff Dahn in Halifax (Canada) to improve batteries for Tesla.

- **Research associate (2021-2022):** I worked as a research associate in the Mark Obrovac lab, also in Halifax.

- **Post-doctoral fellow at CMU (2022-2024):** I then joined Venkat Viswanathan and Jay Whitacre labs at CMU.

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What is a lithium-ion battery?

Batteries are essential to of our economy

Electric cars

Grid energy storage

Portable electronics

And more…

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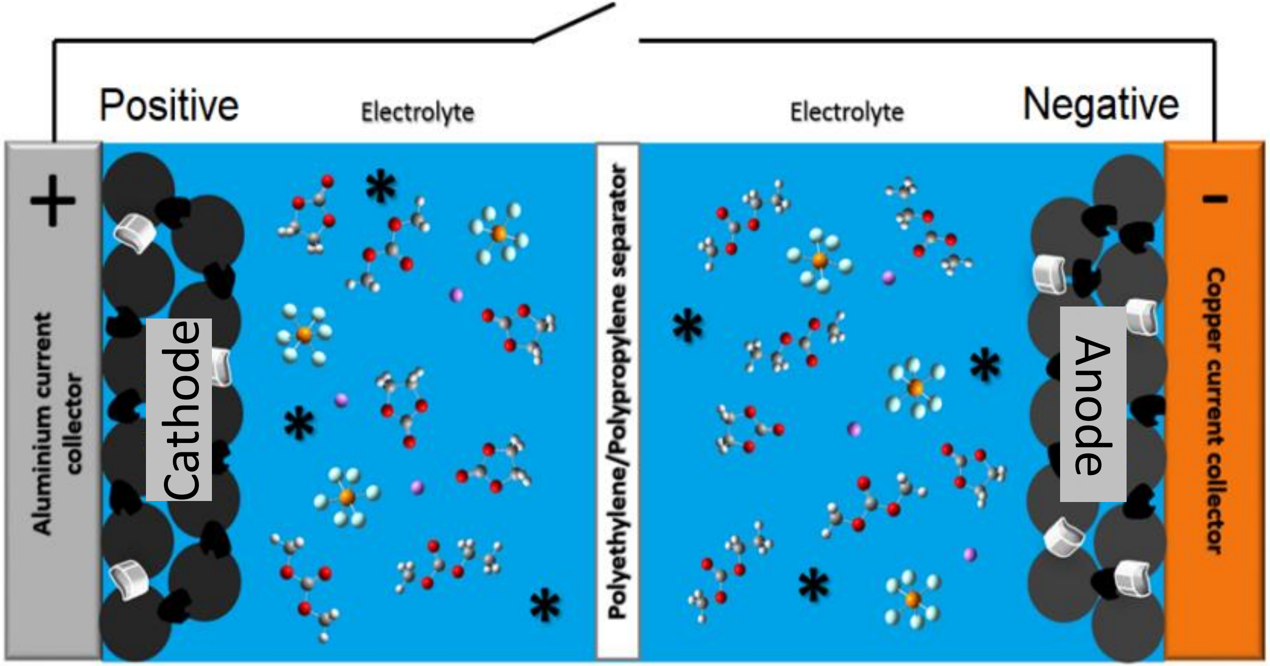
https://www.tesla.com/en_th/model3

https://www.energy-storage.news/tesla-maintains-2030-target-of-1500gwh-annual-energy-storage-deployment/

https://www.abc.net.au/news/2022-09-25/electric-planes-could-see-short-flights-return-regional-cities/101458156

https://innovatsioonipesadest.tehnopol.ee/?g=best-asus-gaming-laptops-in-2023-qq-7ZnvLaFO

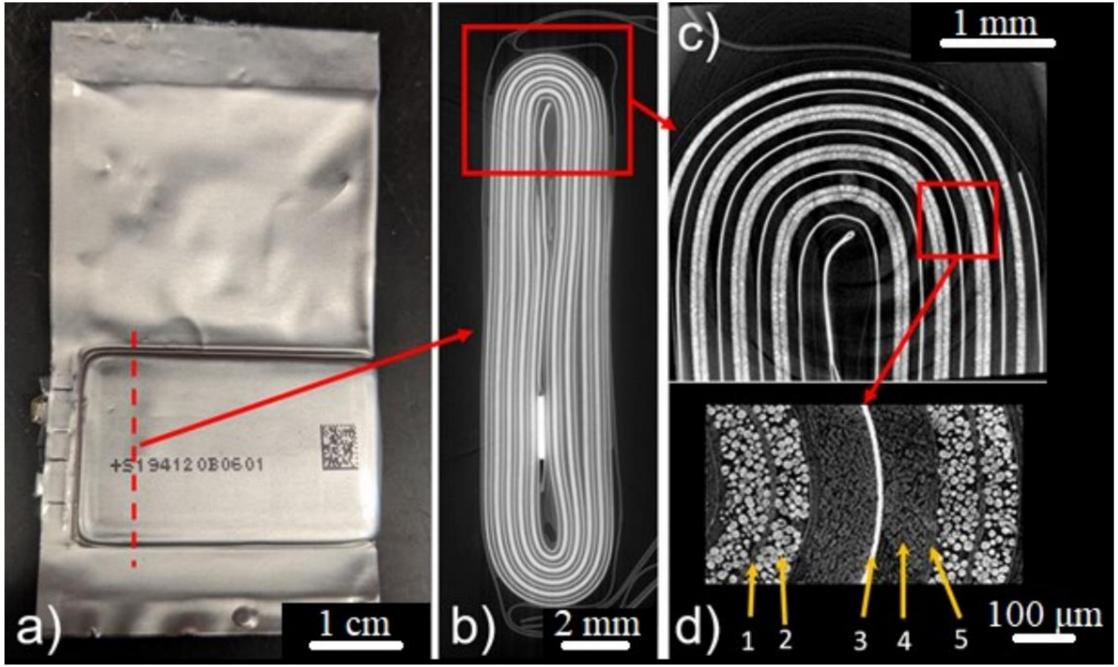
The lithium-ion batteries is a key player in this field.



The electrolyte is a mixture of solvents, additives and one or more salts.

Inside a lithium-ion battery

Pouch cell format



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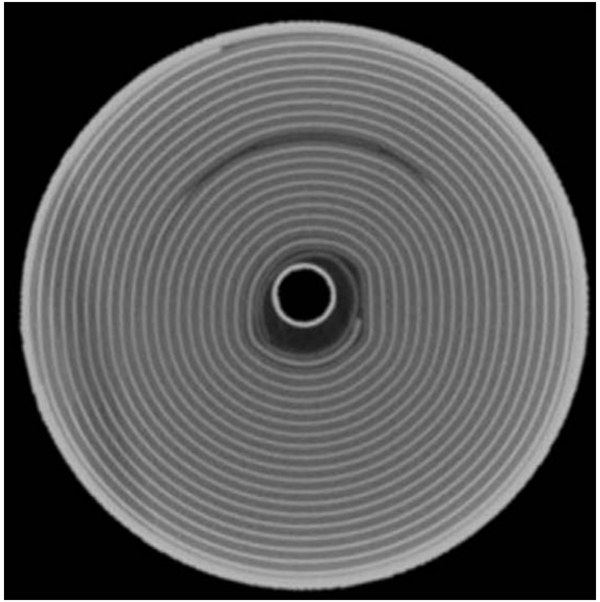
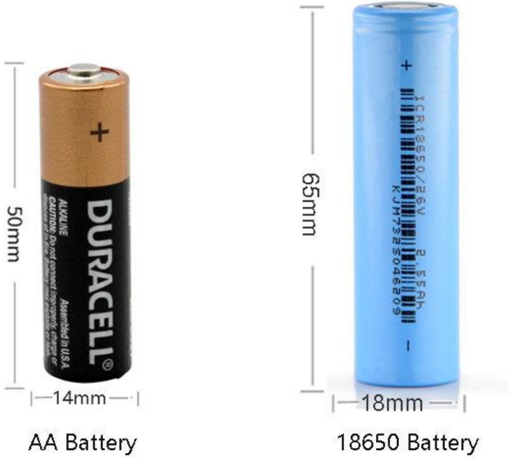
CT-scan courtesy of Toby Bond.

Inside a lithium-ion battery

Cylindrical cell format





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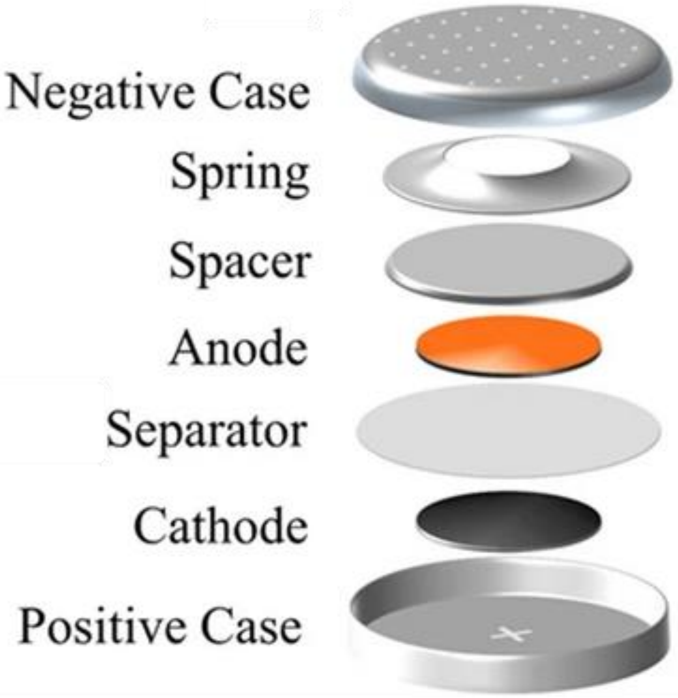
Lisa Willenberg et al 2020 J. Electrochem. Soc. 167 120502 https://www.ecolithiumbattery.com/18650-battery-vs-aa-battery/ https://www.onecharge.biz/lithium-cell-format/

Video : making cylindrical cells

https://www.youtube.com/watch?v=j0dNxDMAtes&ab_channel=GommeBlog.it%3ACar%26Performance&t=0m43s

Inside a lithium-ion battery

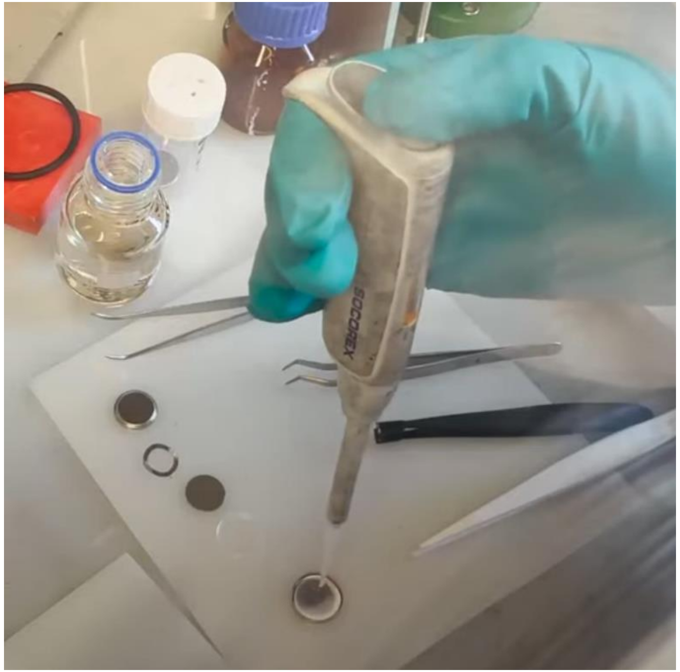
Coin cell format



Ionics **29**, 5285–5293 (2023)

Video : making coin cells

https://www.youtube.com/watch?v=-ppI1xCXL_4&ab_channel=FOMTechnologies&t=2m24s



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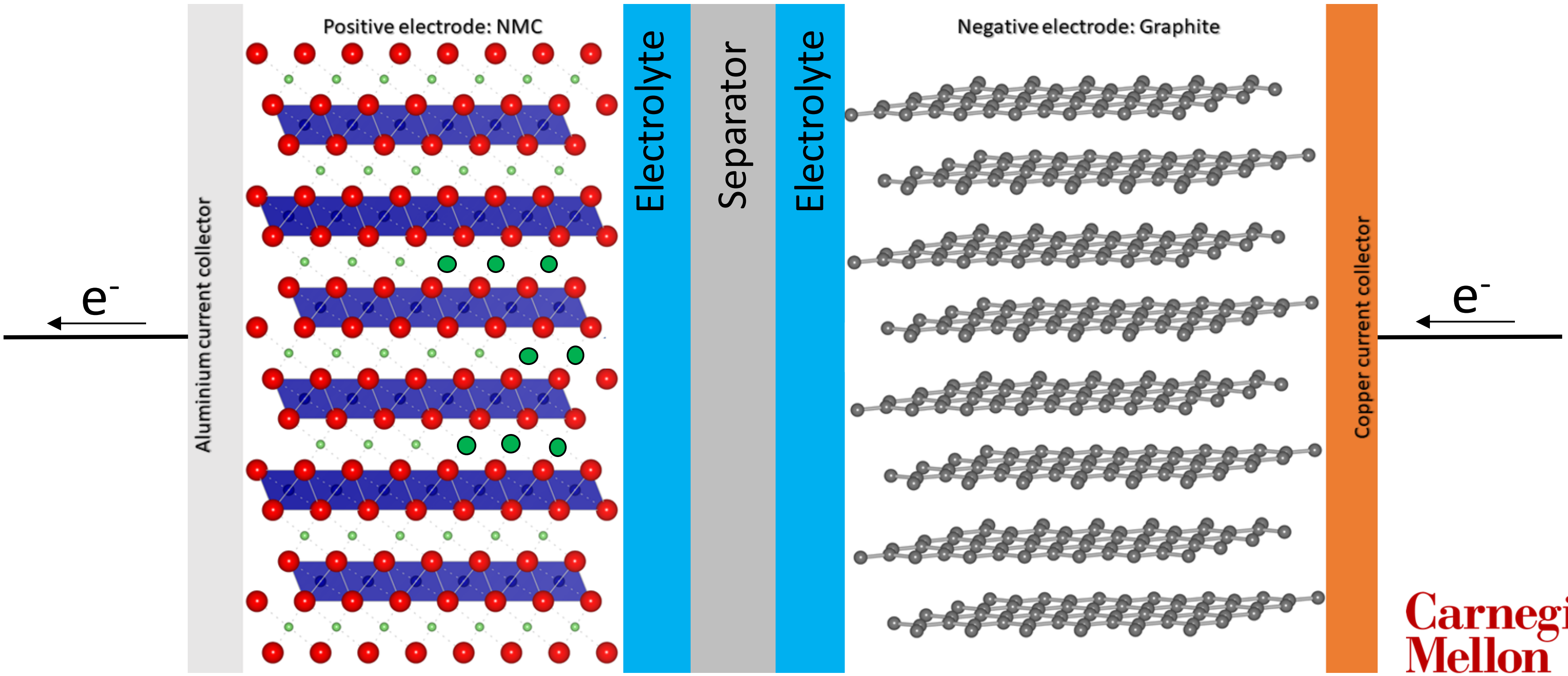
But how does it work?

Charging:

Li-ion batteries charge by converting electrical energy into chemical energy. Li-ions diffuse from the cathode to the anode during this process. Chemical energy is stored at the anode.



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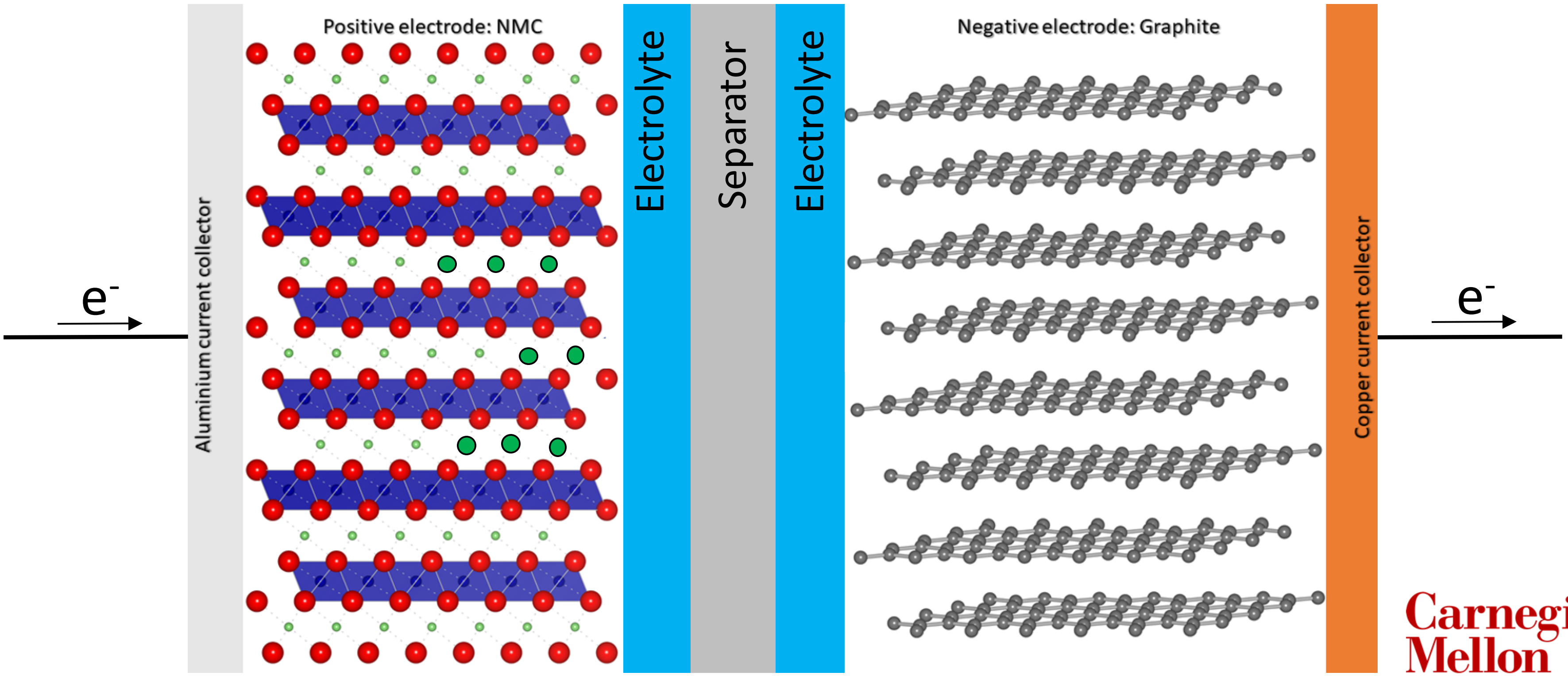
Discharging:

The opposite process occur. If the battery was perfect, it would come back to its original state.



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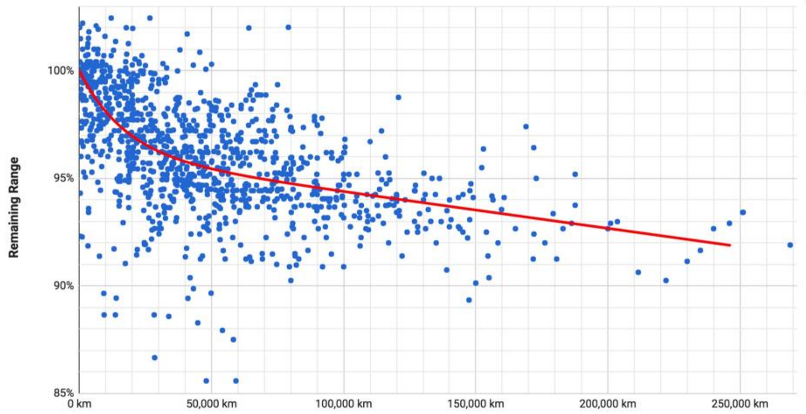
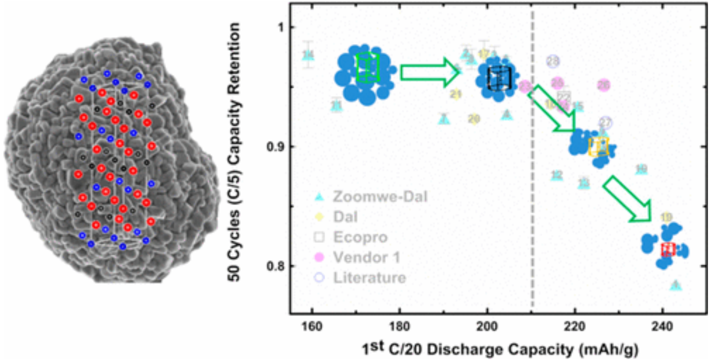
Questions?

But it’s not perfect. Challenges are still present.

Tesla model S/X





Battery degradations: Energy density vs. degradation battle.

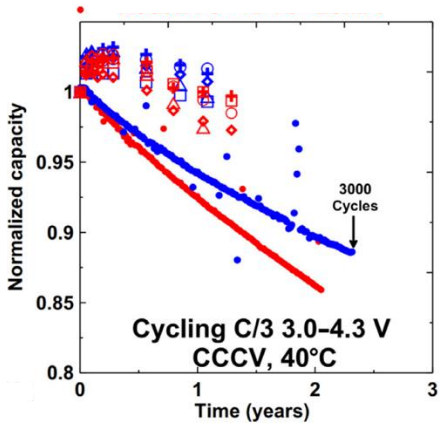
As we strive to extend the range of electric vehicles, it often comes at the cost of higher degradations. This holds true across many battery chemistries.

https://www.teslarati.com/tesla-battery-life-80-percent-capacity-840km-1-million-km/ https://pubs.acs.org/doi/full/10.1021/acs.chemmater.9b02372

Challenges are still present.

The same problem for ultra fast charging

(charging faster than 10 minutes)



Blue: Electrolyte A
Red: Electrolyte A + 20% Methyl acetate (fast charging additive)

Optimizing the battery for faster charging result in more degradation

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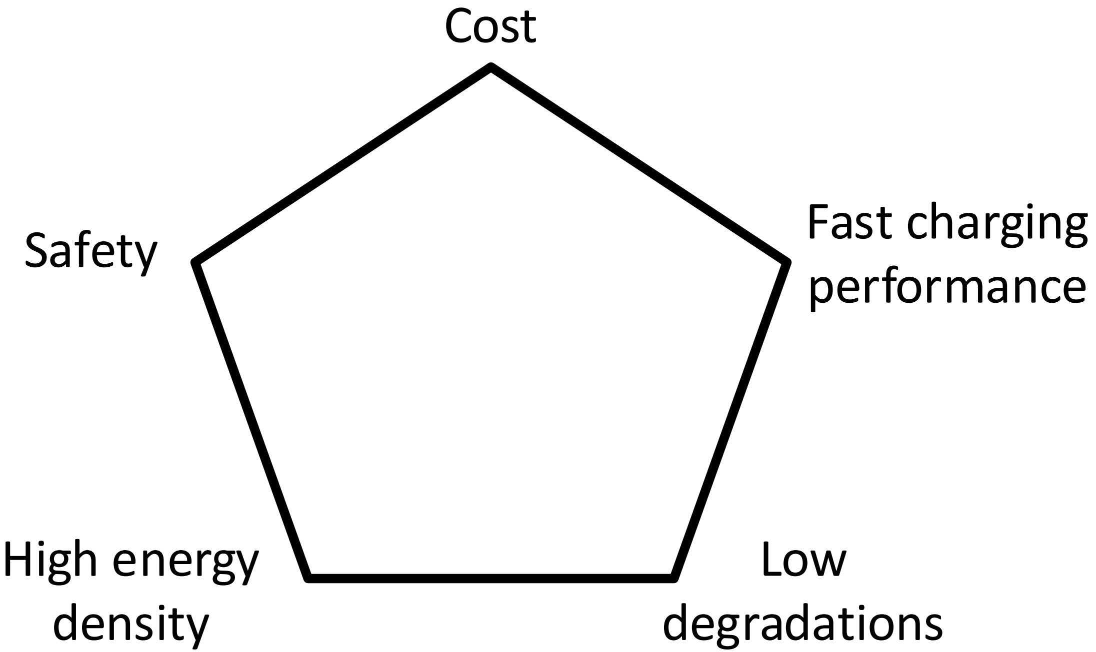
https://www.autotrader.com/car-shopping/tesla-destination-charging-vs-supercharging

Trends in Chemistry, April 2020, Vol. 2, No. 4

The real challenge is to optimize many parameters at the same time.



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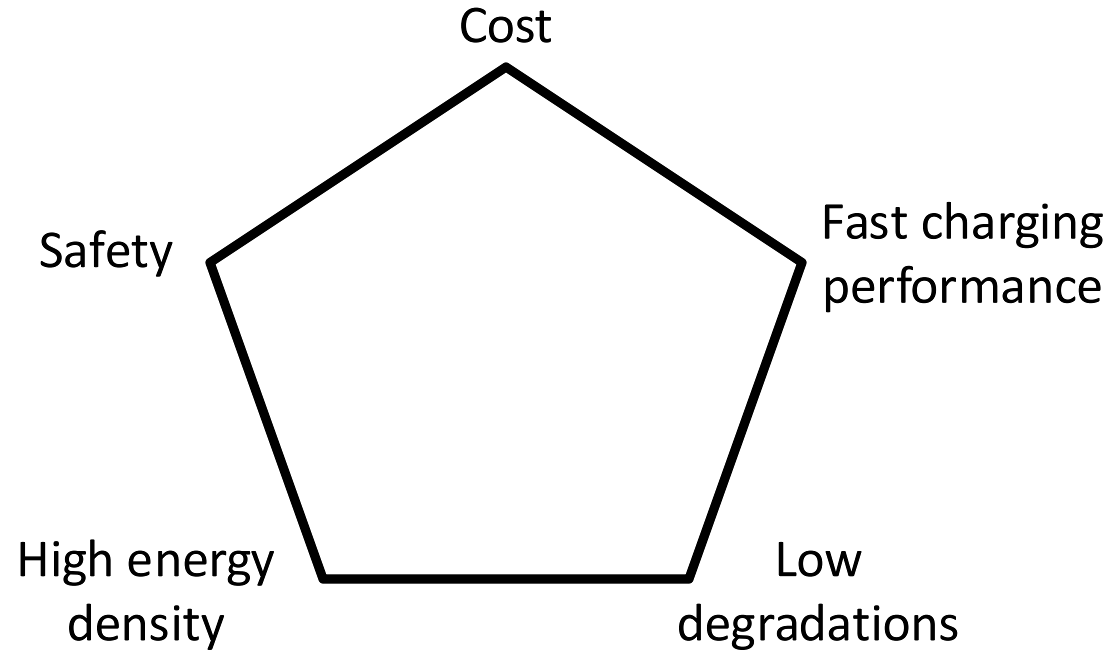
How to do this? History can be a good teacher.



Brief History of anode material

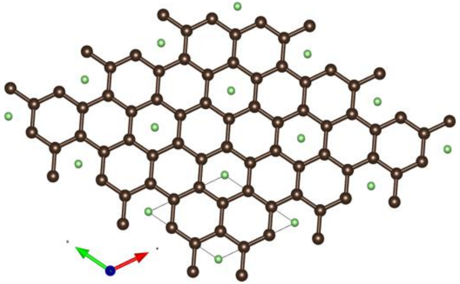
In the 80s, **lithium metal** was used as the anode due to its **high energy density**.

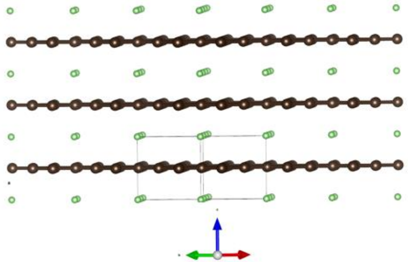
In 1989, a cellphone **caught fire** and caused minor burns to the user. The cause: A battery from Molicel containing **lithium metal as the anode**.

Due to this incident, **graphite eventually replaced lithium metal anode** due to its higher safety, despite its lower energy density. Sony commercialized this technology in 1991.

Lithium metal

Lithiated graphite





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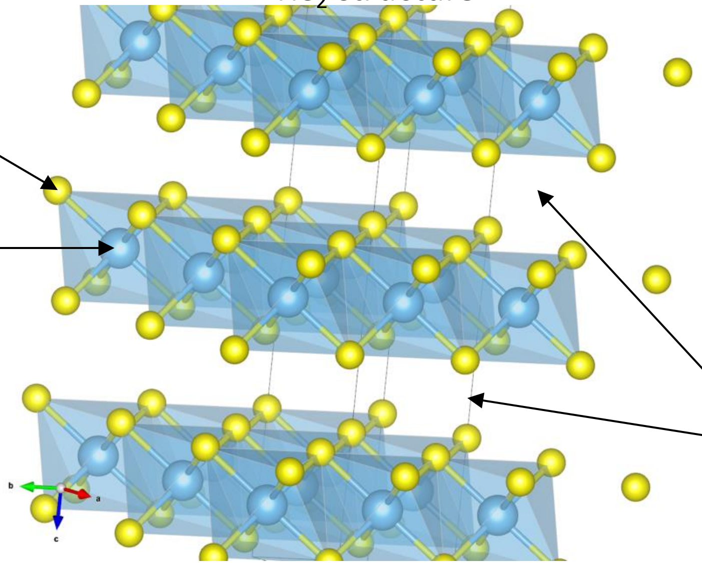
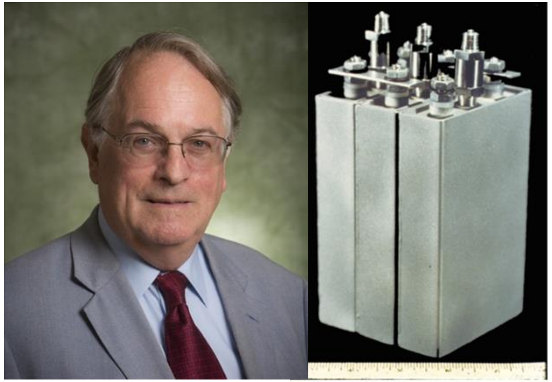
https://www.pnnl.gov/news-media/longer-lived-lithium-metal-battery-marks-step-forward-electric-vehicles https://electricautonomy.ca/ev-supply-chain/batteries/2020-09-18/moli-energy-lithium-battery-technology/

History of cathode material development : $LiTiS_2$

- M. Stanley Whittingham's superconductivity research in the 1970s on layered sulfides led to the foundational work for the first rechargeable lithium battery: The $LiTiS_2$ cathode.

TiS_2 structure





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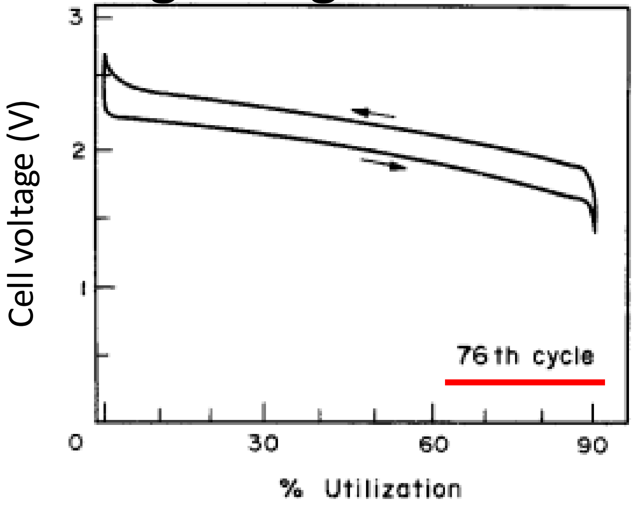
Sibum, H., Güther, V., Roidl, O., Habashi, F., Uwe Wolf, H. and Siemers, C. (2017). Titanium, Titanium Alloys, and Titanium Compounds. In Ullmann's Encyclopedia of Industrial Chemistry, (Ed.).

However, the battery had low average voltage resulting in lower energy density.

Average voltage at beginning of life : 1.9 V



Volumetric energy density =
1/Volume x Capacity (mAh) x Average voltage

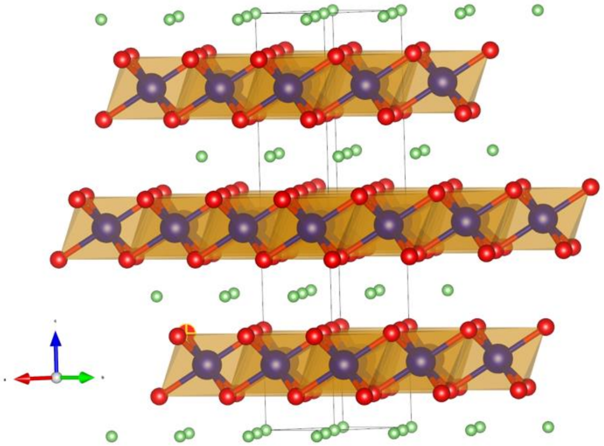
Specific energy density =
1/Mass x Capacity (mAh) x Average voltage

1 mAh = 3.6 Coulombs

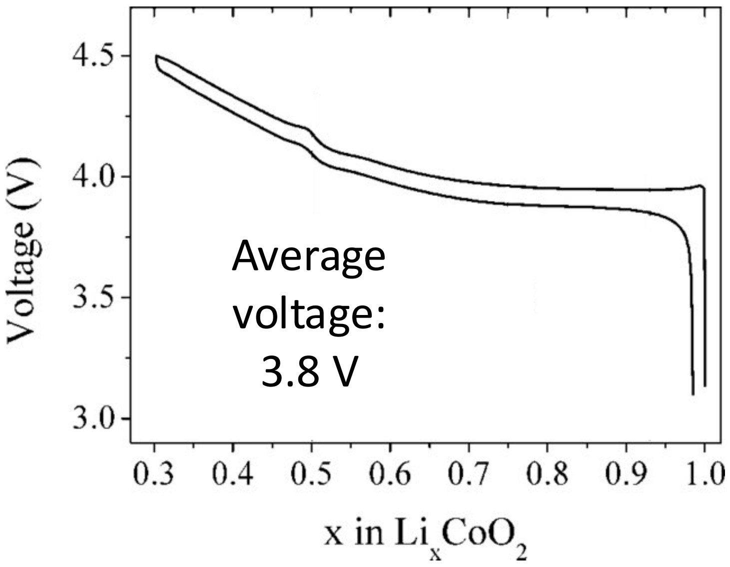
Questions?

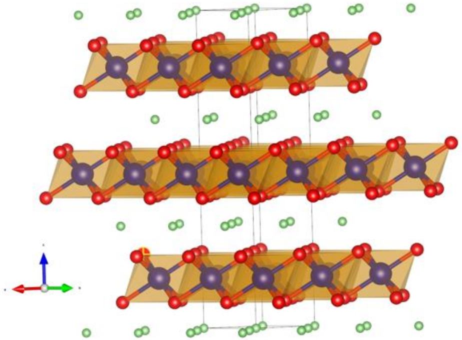
History of cathode material development: $LiCoO_2$

- In the 1980s, John Goodenough's exploration of $LiCoO_2$, inspired by its similar structure to $LiTiS_2$, revealed its superior energy storage capabilities, setting the stage for the first commercial lithium-ion battery by Sony.



History of cathode material development: $LiCoO_2$





The higher average voltage is caused by the stronger Li - O bonds compared to the weaker Li - S bonds.

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Modified from *Chem. Mater.* 2008, 20, 2, 583–590

History of cathode material development: $LiNi_xMn_yCo_{1-x-y}O_2$ (NMC)

- Cobalt is expensive. For this reason, cheaper option than $LiCoO_2$ where needed.
- While $LiNiO_2$ and $LiMn_2O_4$ are cheaper, LiNiO2 is also very unsafe and $LiMn_2O_4$ has low energy density.
- In 2001, on the way back from a Conference, Jeff Dahn and Zhonghua Lu thought about mixing nickel, manganese and cobalt to make $LiNi_xMn_yCo_{1-x-y}O_2$ (NMC). This resulted in a major leap towards cost-effective and safe cathodes with higher capacities.
- Today, NMC is still used as a cathode material in many product.

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Small Methods 2020, 4, 2000039

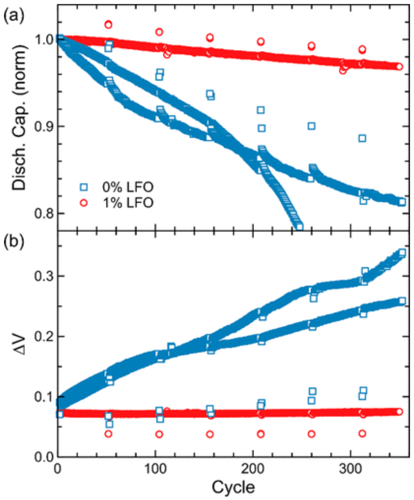
What are some ways that energy density can be improved?

1. At the cathode, increase the average voltage and/or the amount of lithium that can be stored.
2. At the anode, keep the average voltage low and/or increase the amount of lithium that can be stored
3. More efficient battery design (thicker electrodes, etc.).

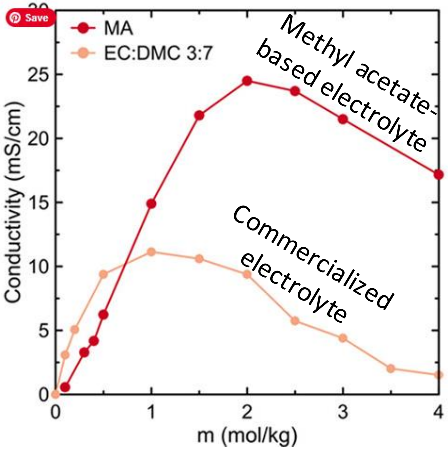
https://www.kaltire.com/en/why-should-you-keep-your-gas-tank-full.html

We need to keep degradations, fast charging and safety in mind. Electrolyte additives or electrolyte reformulation can help.

Additives can decrease degradations

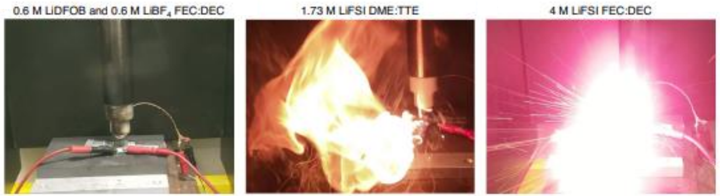


Electrolyte reformulation can increase conductivity, enabling faster charging.



Salt concentration

Electrolyte reformulation can increase safety.



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ACS Appl. Mater. Interfaces 2019, 11, 15, 14095–14100
J. Phys. Chem. C 2020, 124, 23, 12269–12280
Nature Energy volume 5, pages 693–702 (2020)

And cost.

Cost can be decreased by improving the energy density of the battery.

Less material is needed to store the same amount of energy, so $/kWh is lower.

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https://www.lipobatteries.net/product/li-ion-battery-18650a-3500mah-100pcs/

In summary

- Energy density can be increased by adjusting the average voltage and amount of lithium atoms stored in each electrodes. Increasing the energy density result in lower cost ($/kWh lower).
- The rate of the degradation can be decrease by adding electrolyte additives.
- The fast-charging capability and safety of batteries can be improved using electrolyte reformulation.

Questions?