LITHIUM-ION BATTERIES

SELF-HEALING CHEMISTRY TO THE RESCUE!

Elior Bilow, Matthew Blau, Joshua Dweck & Elena Gomel
Prof. Yair Ein-Eli & Moran Balaish Ph.D (Material Sciences)

Introduction

Lithium-ion batteries are used in most energy sectors. They are comprised of an anode (commonly graphite), cathode and electrolyte (Figure 1). During discharge, the lithium cations move from the negative electrode to the positive electrode, forming a lithium compound, while the electrons flow in the same direction. When charging, the reverse occurs. Silicon shows great promise as an anode, as it has 10x the capacity of graphite. However, due to the higher capacity, there is a large volume variation in the Si-based anode upon charging and discharging (lithiation and delithiation), causing cracking (pulverisation) and delamination, which impairs the batteries. We investigated self-healing polymers (Figure 2) as a solution.

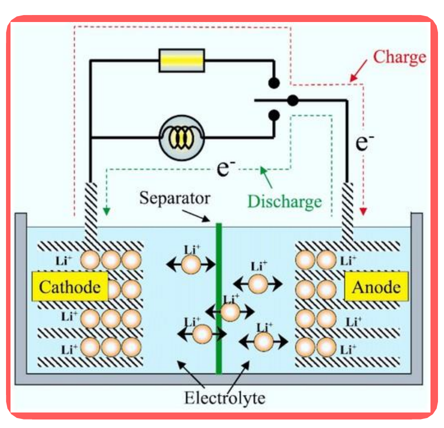


Figure 1. A schematic illustration of the operation of a Lithium-Ion battery. (1)

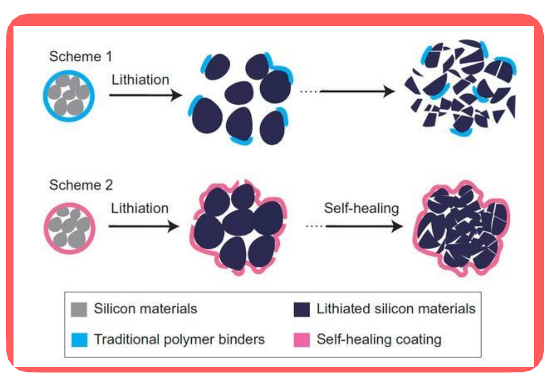


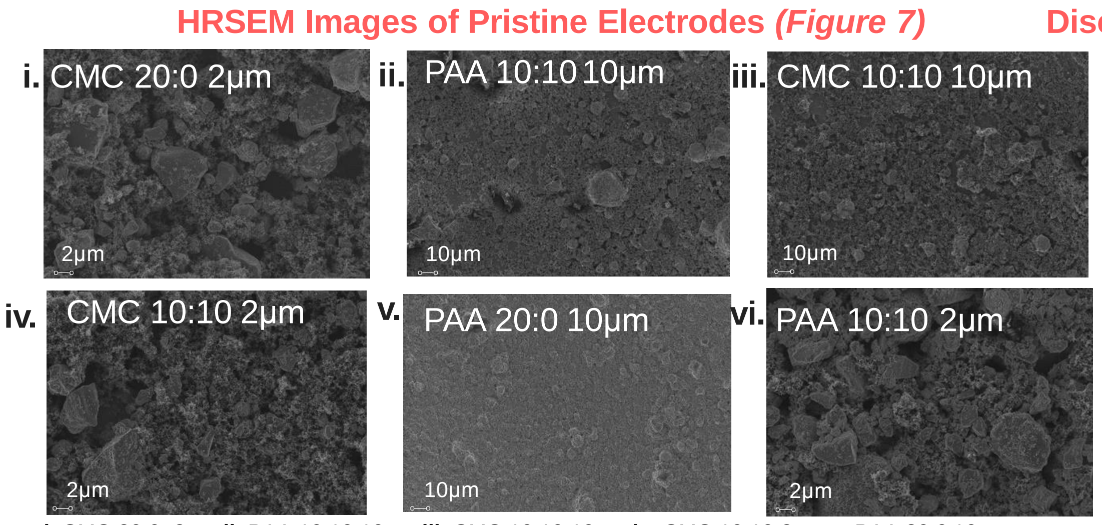
Figure 2. An illustration of the self-healing damage mechanism vs traditional polymer binders during the process of lithiation. (2)

Goals

To produce functioning electrodes and to develop and test hybrid polymers that bind Silicon and Carbon, preventing mechanical fracture and maintaining the electrode structure over repeatable cycling processes.

Results & Observations

HRSEM Images of Pristine Electrodes *(Figure 7)*



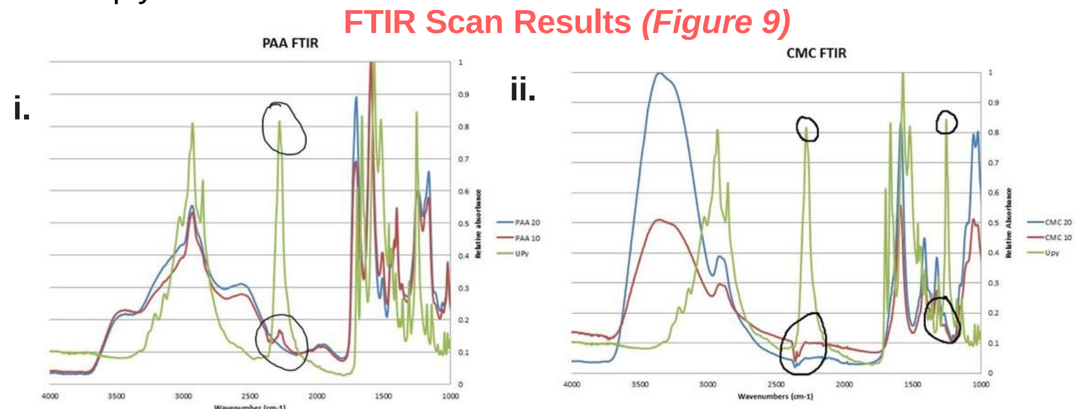
i. CMC 20:0 2μm **ii.** PAA 10:10 10μm **iii.** CMC 10:10 10μm **iv.** CMC 10:10 2μm **v.** PAA 20:0 10μm **vi.** PAA 10:10 2μm

An HRSEM scans a focused electron beam over a surface, creating an image. The electrons interact with the sample, producing signals that provide information about the surface topography and composition.

Observations:

- The PAA 10:10 electrodes had more large clumps than the CMC electrodes and larger clumps than the PAA 20:0.
- The large clumps indicate that the UPy bonded well with the PAA, as UPy was the only difference between the two PAA electrodes
- The CMC 10:10 also has fewer large clumps, showing that the UPy simply did not bond as well to the CMC

FTIR Scan Results *(Figure 9)*

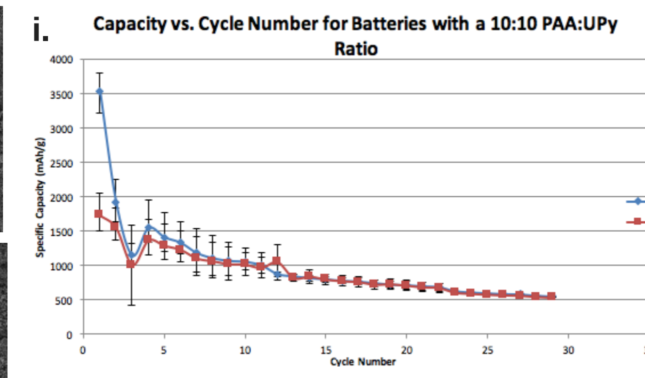


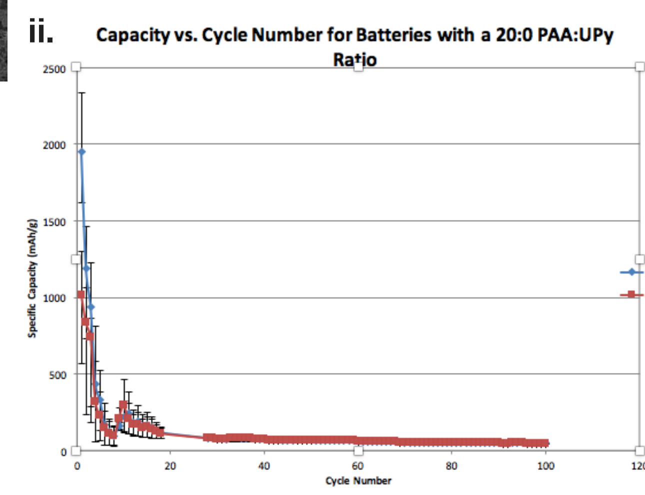
FTIR is a technique used to identify organic materials. This measures the absorption of infrared radiation by the sample material versus wavelength. This information helps identify molecular components and structures.
i. PAA. ii. CMC

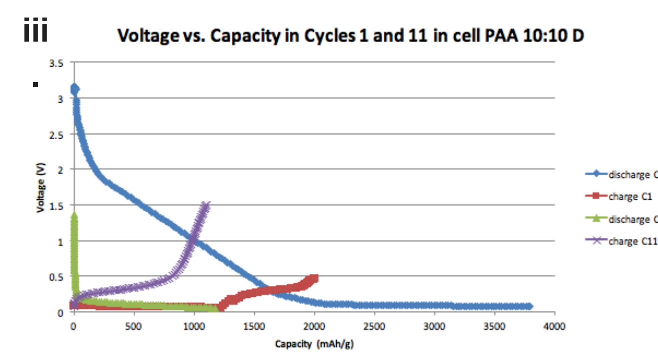
Observations:

- The UPy peak is at 2350 wavenumbers.
- It is not so in the graphs of CMC 20:0 and CMC 10:10, showing that the UPy and CMC mixture was not homogenous.
- The peak is in the PAA 10:10 graph and not in PAA 20:0, showing that the UPy and PAA created a homogenous mixture, allowing for better capacity retention.

Discharge & Charge Results ARBIN *(Figure 8)*







- i. Capacity vs. Cycle number for Batteries with a 10:10 PAA:UPy Ratio. ii. Capacity vs. Cycle number for Batteries with a 20:0 PAA:UPy Ratio. iii. Voltage vs. Capacity in Cycles 1 and 11 in cell PAA 10:10 D

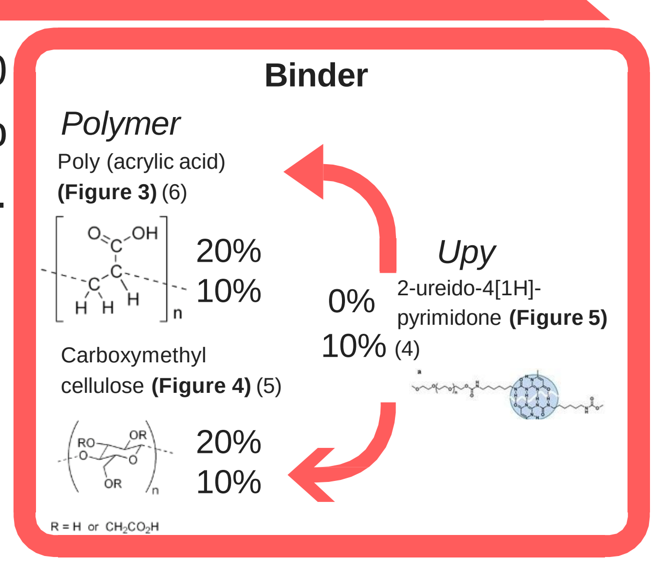
Observations:

Average capacity after 11 cycles:

- PAA 10:10 ≈ 27%
- PAA 20:0 ≈ 10%
- The batteries with a 10:10 PAA: UPy ratio began with and maintained the highest capacity.

Materials

- ***Working electrode:*** Mixture of Si nanoparticles (300 nm), Carbon Black and binder in a 60:20:20 weight ratio
- ***Binders:*** PAA, CMC, and UPy in 20:0 and 10:10 ratios.
- ***Counter electrode***: 11.55 mm diameter Lithium discs.
- ***Electrolyte***: 1M lithium hexafluorophosphate (LiPF6) in ethylene carbonate (EC and dimethyl carbonate (DMC) (1:1 v/v). 0.8 mL
- Battery cell: T-cell (Figure 6)



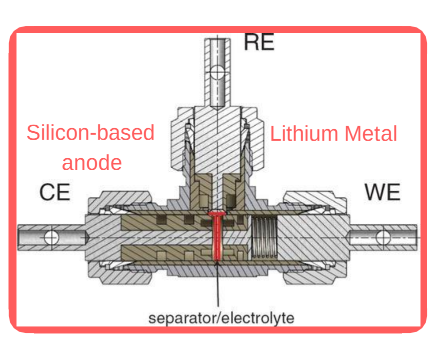


Figure 6. An electrochemical test cell used for evaluation of the electrochemical performance of battery electrodes (3).

Method

i. Fourier Transform Infrared Spectroscopy (FTIR)

Using the FTIR analysis method to scan test samples and observe chemical properties using infrared light.

ii. High-Resolution Scanning Electron Microscopy (HRSEM)

Scanning electrodes to determine surface characterisation.

iii. Discharge & Charge Experiments

Applying constant current to the cells, measuring voltage as a function of time.

***Current = 0.2Amps/Gram*Weight of Si Based on 1'C-Rate' = 4Amps/Gram**

i = 0.2Alg*WSi
1C = 4Alg
(Refer above *)

Conclusions

- PAA is a linear molecule with two possible sites for Hydrogen bonds (Oxygen atoms). CMC has more such sites, but it has a circular structure, making hydrogen bonds weaker or impossible to form (as seen in Figs. 3-4).
- PAA 10:10 had a higher capacity and retained more of its capacity than the other electrodes that we tested. (as seen in Figs. 7-9)
- The UPy does not work by itself because it does not create the long chains necessary to bind the Silicon and Carbon (as seen in Fig. 5).

Future Work

- Continue to explore the optimal weight ratio and polymer type in order to prevent mechanical fracture and allow for batteries with the greatest possible capacity and capacity retention.
- Investigate polymers with a linear structure and more Oxygens, which could create even more bonds with the UPy, allowing for even higher capacity and greater capacity retention.

References

1. "Schematic Battery - The Wiring Diagram." Readingrat.net, 18 May 2017.
2. Mazouzi, D. "Researchgate.net, Apr. 2015.
3. Electrochemical Test Cells Used for Evaluation of Electrochemical Performance of Battery Electrodes." Scientific Reports, 2017.
4. Da Greef, Tom F.A. 7 May 2008.
5. Carboxymethyl cellulose, Wikipedia, 30 July 2017
6. Poly(Acrylic Acid). Wikipedia, 25 Dec. 2016.

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