



# A Mechanistic Investigation of the Relationship Between Battery Energy and Capacity

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# Relating Capacity and Energy Losses

## Are capacity and energy loss equivalent?

“Capacity” is one of the most critical metrics in energy storage system standards.

However, there is inconsistency in the definition of capacity across documents.

Some standards refer to an energy capacity with units of Wh and a coulombic capacity with units of Ah

Other standards simply use the term ‘capacity’ without defining the units and use it on a normalized base.

Can the Wh and Ah definitions be used interchangeably?

$$Capacity_i(Ah) = \underset{\substack{\uparrow \\ \# \text{ of } e^-}}{n} \cdot \overset{\substack{\downarrow \\ \text{Faraday number} \\ \text{Charge on } 1 e^-}}{F} \cdot \underset{\substack{\uparrow \\ \# \text{ of moles}}}{N} = \int_0^t Current \cdot dt$$

Definition: Total amount of electrons a battery can store, independent of its voltage.

Units: Ampere-hours (Ah)

What it means: A 10 Ah phone battery can theoretically hold 10 A of current for 1 hour

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$$Energy_i(Wh) = \int_0^t Voltage \cdot Current \cdot dt \\ = \overline{Voltage} \cdot Capacity$$

Definition: Actual electrical work the battery can deliver.

Units: Watt-hours (Wh)

What it means: A 10Ah 12V battery holds 120Wh of energy.

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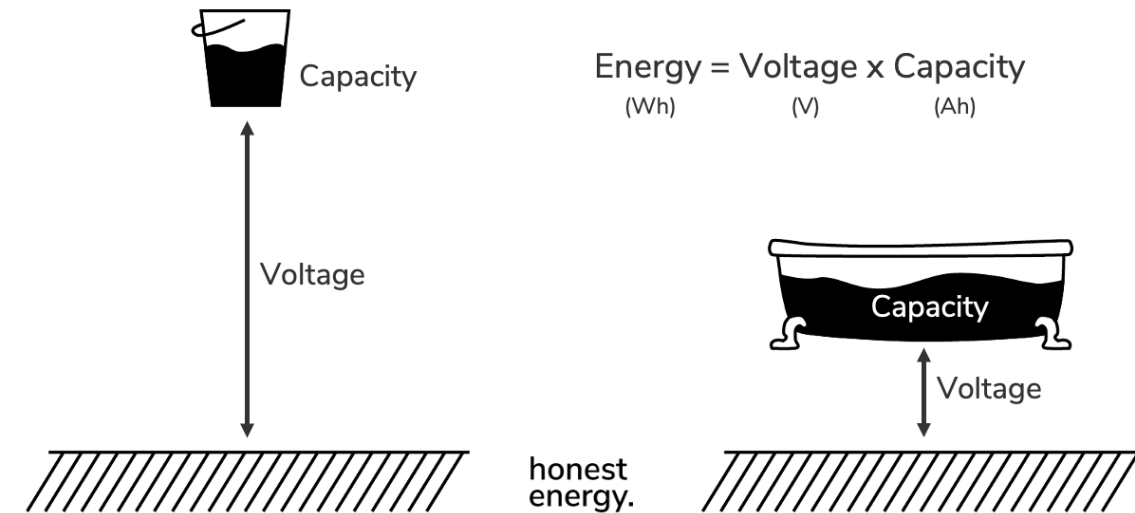
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$$\begin{aligned} \text{Capacity}_i(\text{Ah}) &= \overset{\substack{\text{Faraday number} \\ \text{Charge on } 1 \text{ e}^-}}{n \cdot F \cdot N} = \int_0^t \text{Current} \cdot dt \\ &\quad \uparrow \quad \quad \uparrow \\ &\quad \text{\# of e}^- \quad \text{\# of moles} \\ \text{Energy}_i(\text{Wh}) &= \int_0^t \text{Voltage} \cdot \text{Current} \cdot dt \\ &= \overline{\text{Voltage}} \cdot \text{Capacity} \end{aligned}$$



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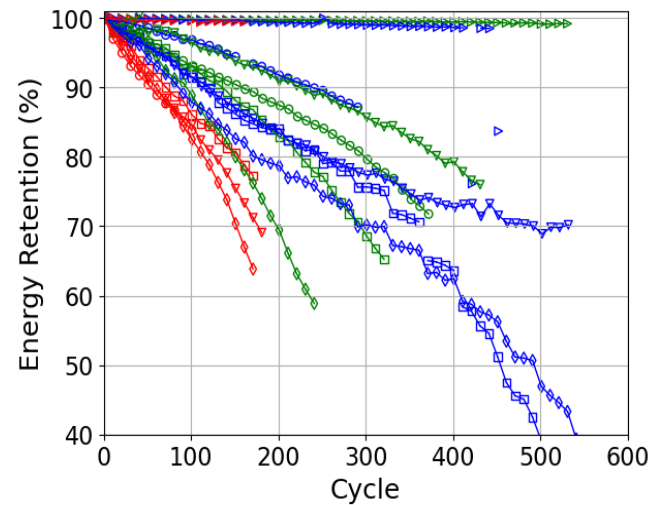
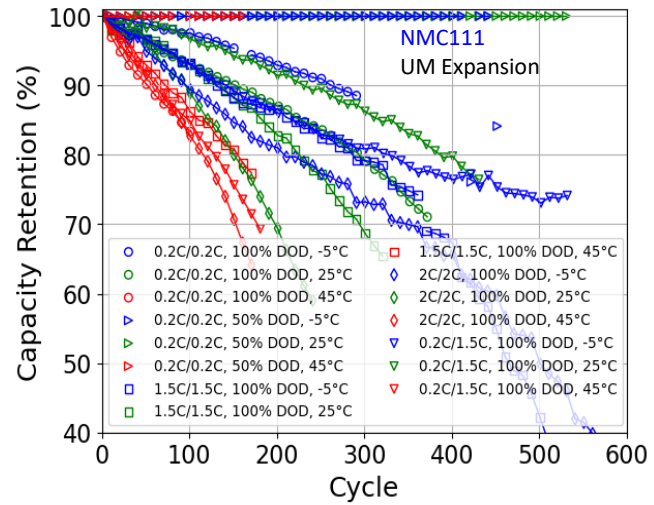
$$\text{Capacity Retention}_i (\%) = \frac{\text{Capacity}_i (\text{Ah})}{\text{Capacity}_0 (\text{Ah})} \times 100\%$$

$$\text{Energy Retention}_i (\%) = \frac{\text{Energy}_i (\text{Wh})}{\text{Energy}_0 (\text{Wh})} \times 100\% = \frac{\text{Capacity}_i (\text{Ah}) \times \overline{\text{Voltage}}_i (\text{V})}{\text{Capacity}_0 (\text{Ah}) \times \overline{\text{Voltage}}_0 (\text{V})} \times 100\%$$

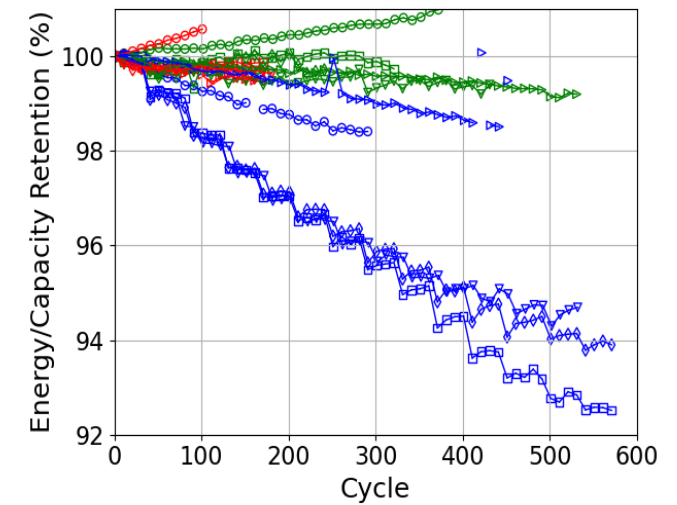
# Relating Capacity and Energy Losses

## Are capacity and energy loss equivalent?

Experimental observations from available battery databases



Both seem to follow similar trends



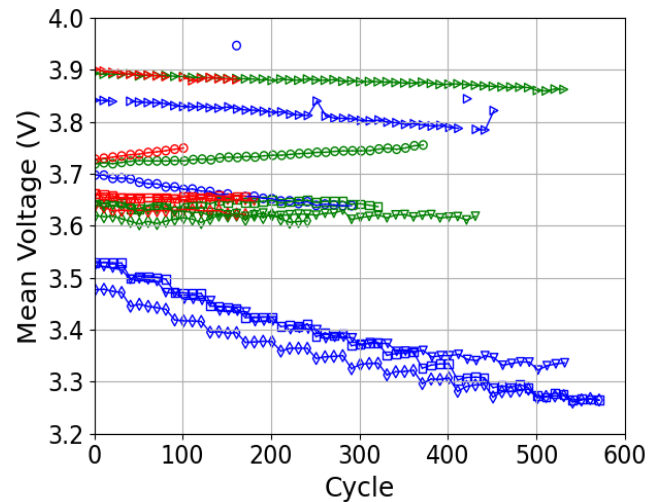
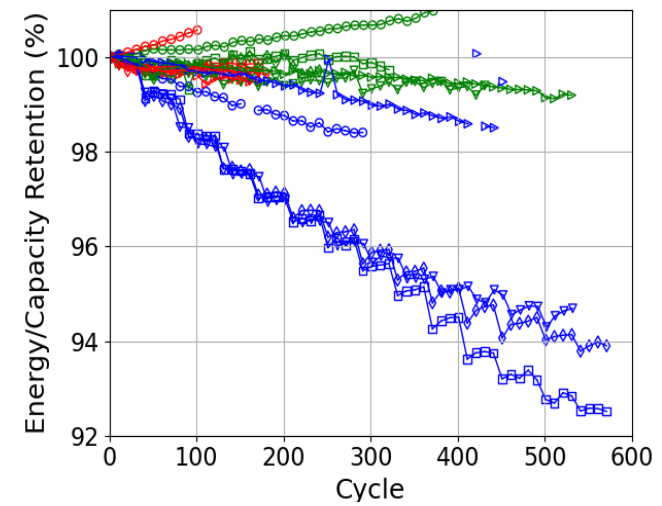
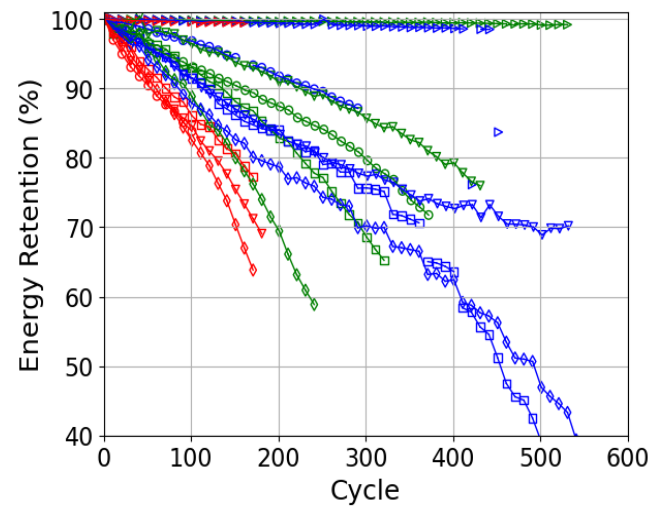
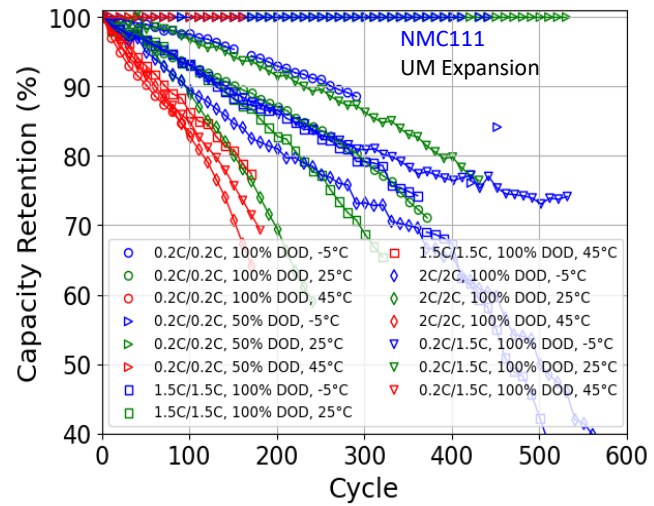
Clearly not that simple...

$$\frac{E}{Q} = \frac{\text{Energy Retention}_i (\%)}{\text{Capacity Retention}_i (\%)}$$

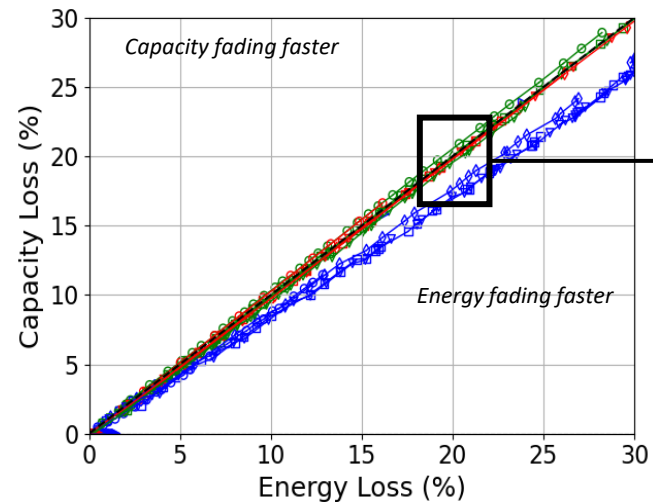
# Relating Capacity and Energy Losses

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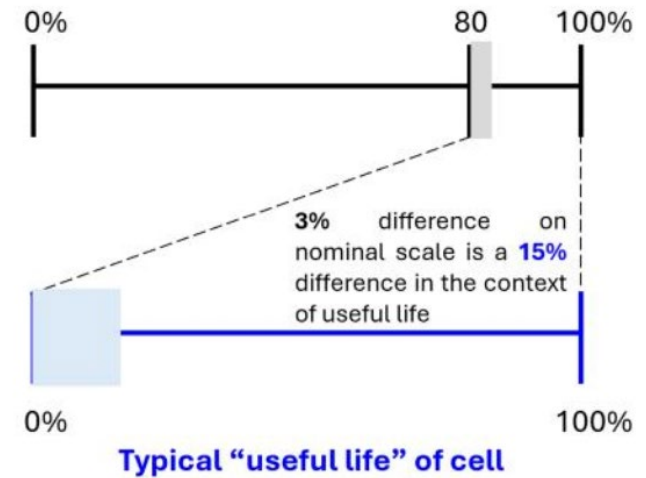
Experimental observations from available battery databases



Why?

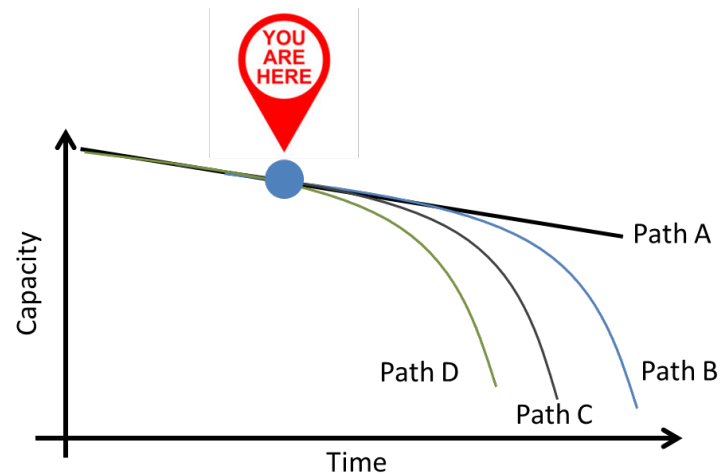


Nominal capacity or energy of cell



# The complexity of battery degradation

## Path dependence of the degradation



Charging



Temperature



Discharging



Different paths will lead to different degradations

Every battery is different → Different voltage variations

# The complexity of battery degradation

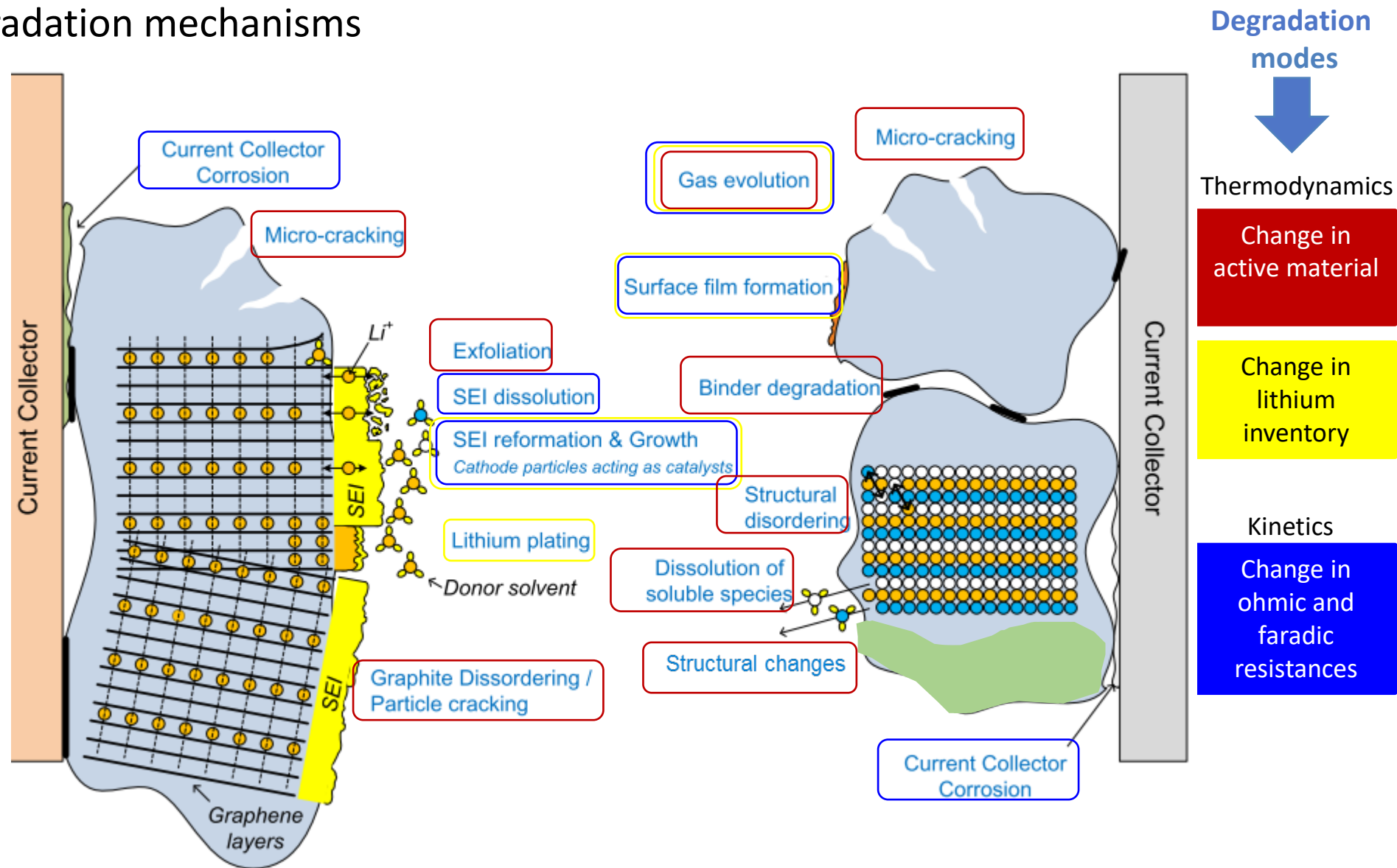
## A million ways to fail...

### Lithium-ion battery degradation mechanisms

20+ possible mechanisms

- Positive Electrode
- Negative Electrode
- Separator
- Electrolyte
- Current collectors
- Complex mix

Degradation modes refer to **the impact of a mechanism rather than its root cause.**



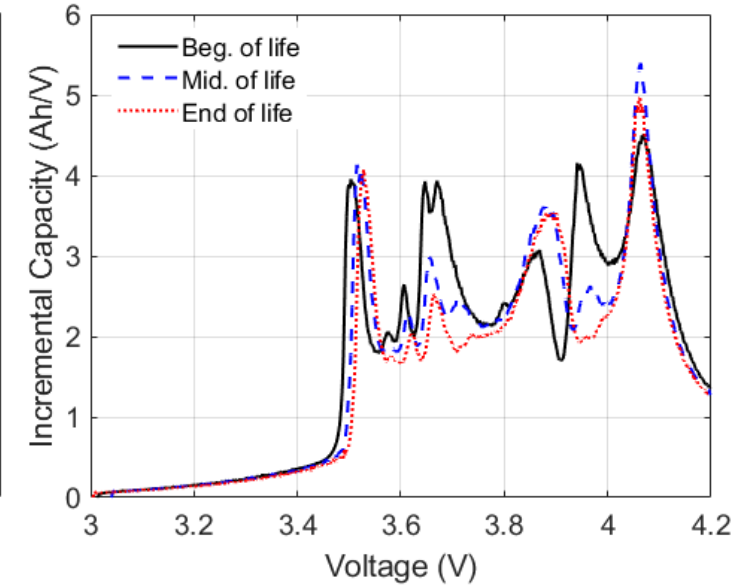
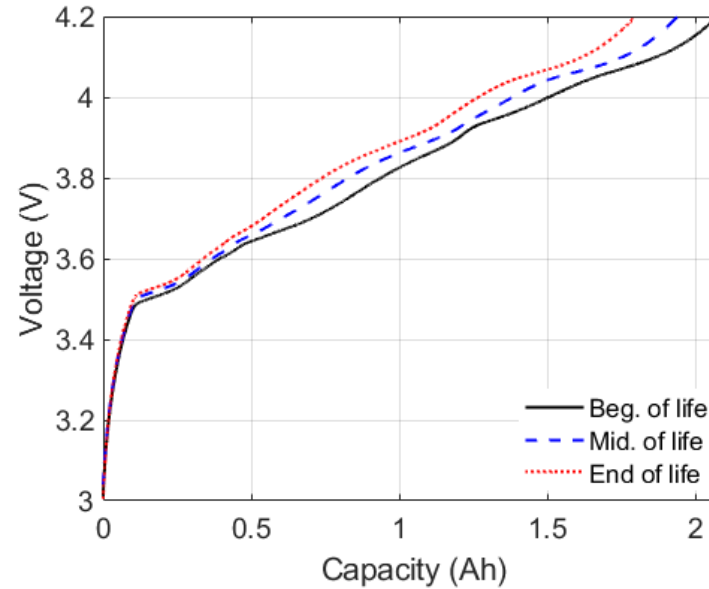
# The complexity of battery degradation

## How to visualize minute voltage changes?

Evolution of the voltage response

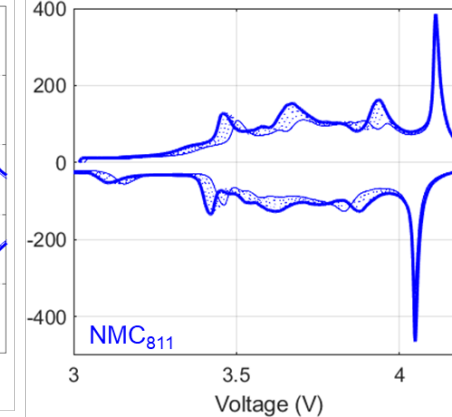
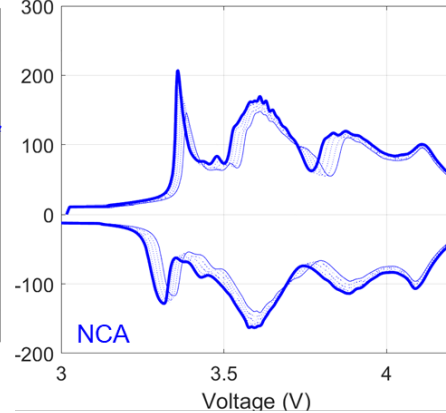
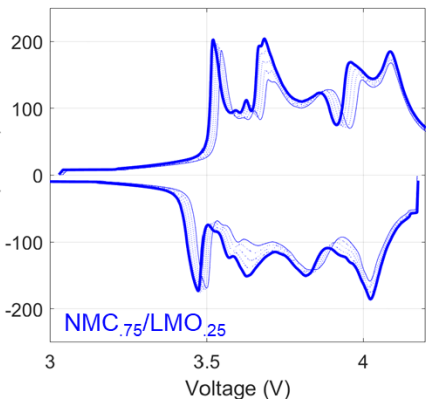
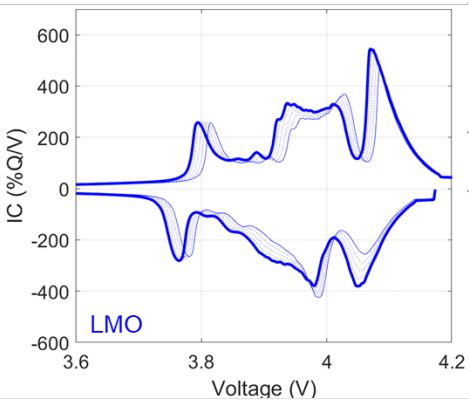
Degradations will affect voltage differently

Use of derivative curves to enhance changes



Response is chemistry dependent

Li-ion or Na-ion

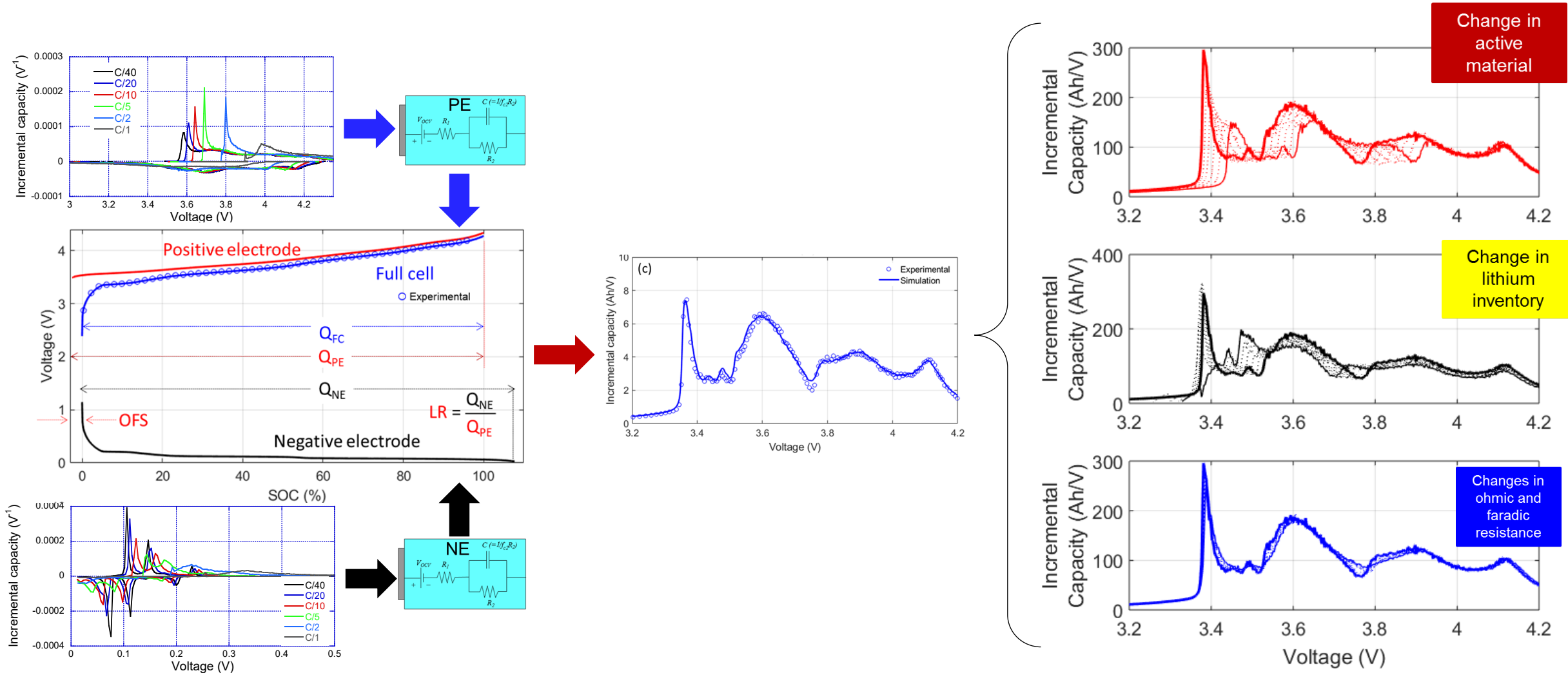


Need a model to relate voltage changes to degradation modes and to track their evolution

# Relating Capacity and Energy Losses

## Individual Electrode Performance

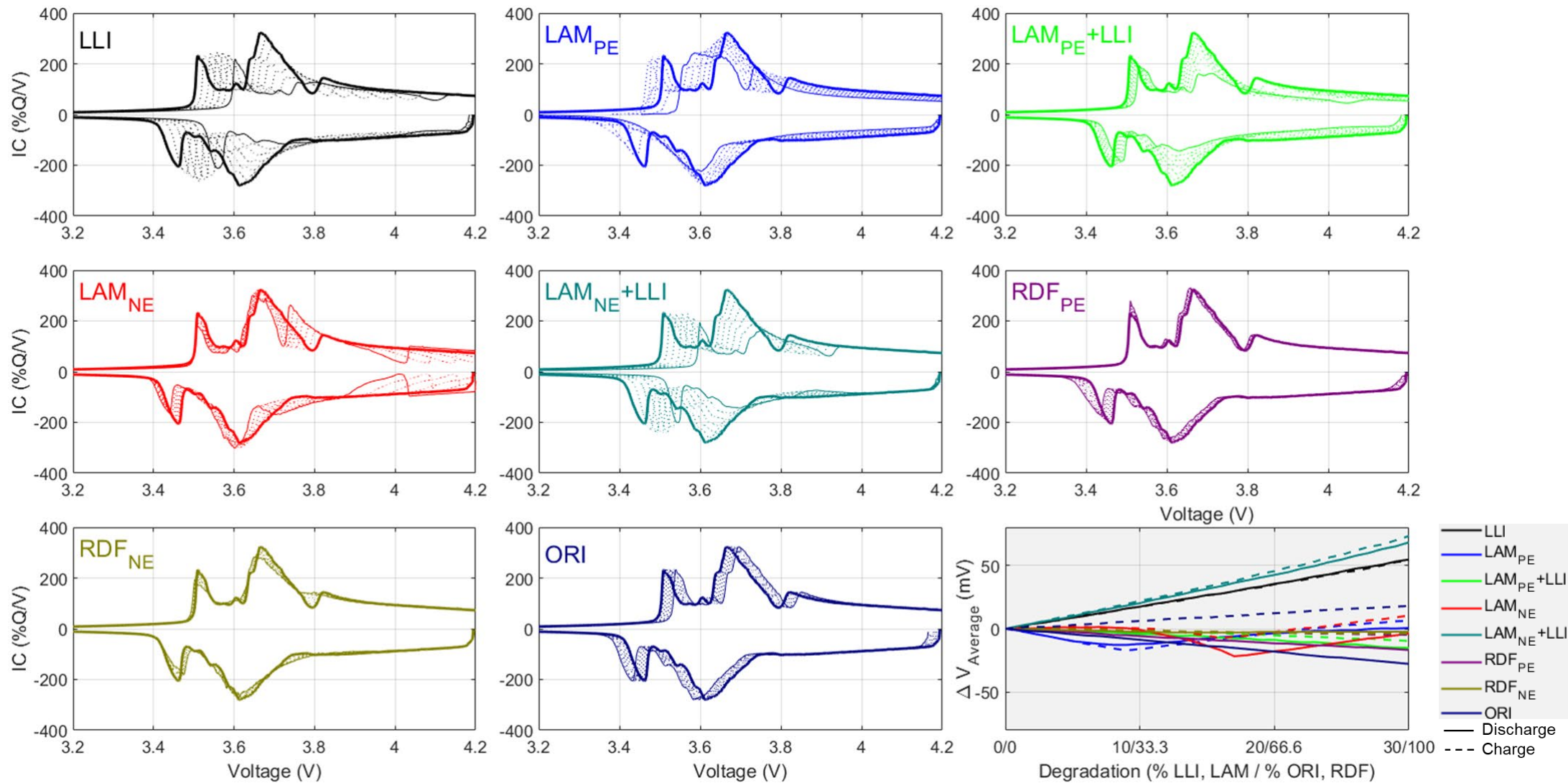
### Emulation of the full-cell response from half-cell data



# Relating Capacity and Energy Losses

## Individual Electrode Performance

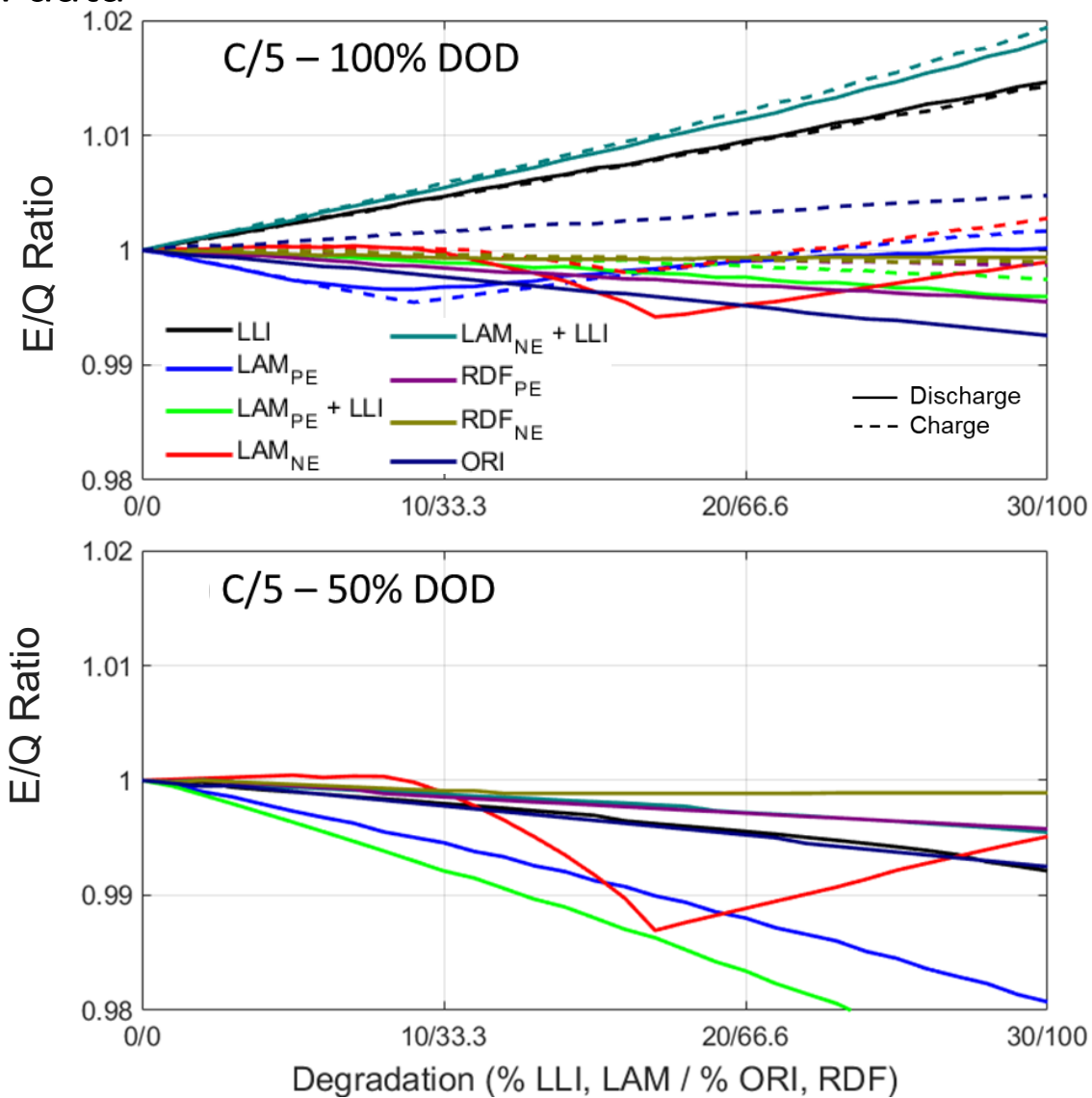
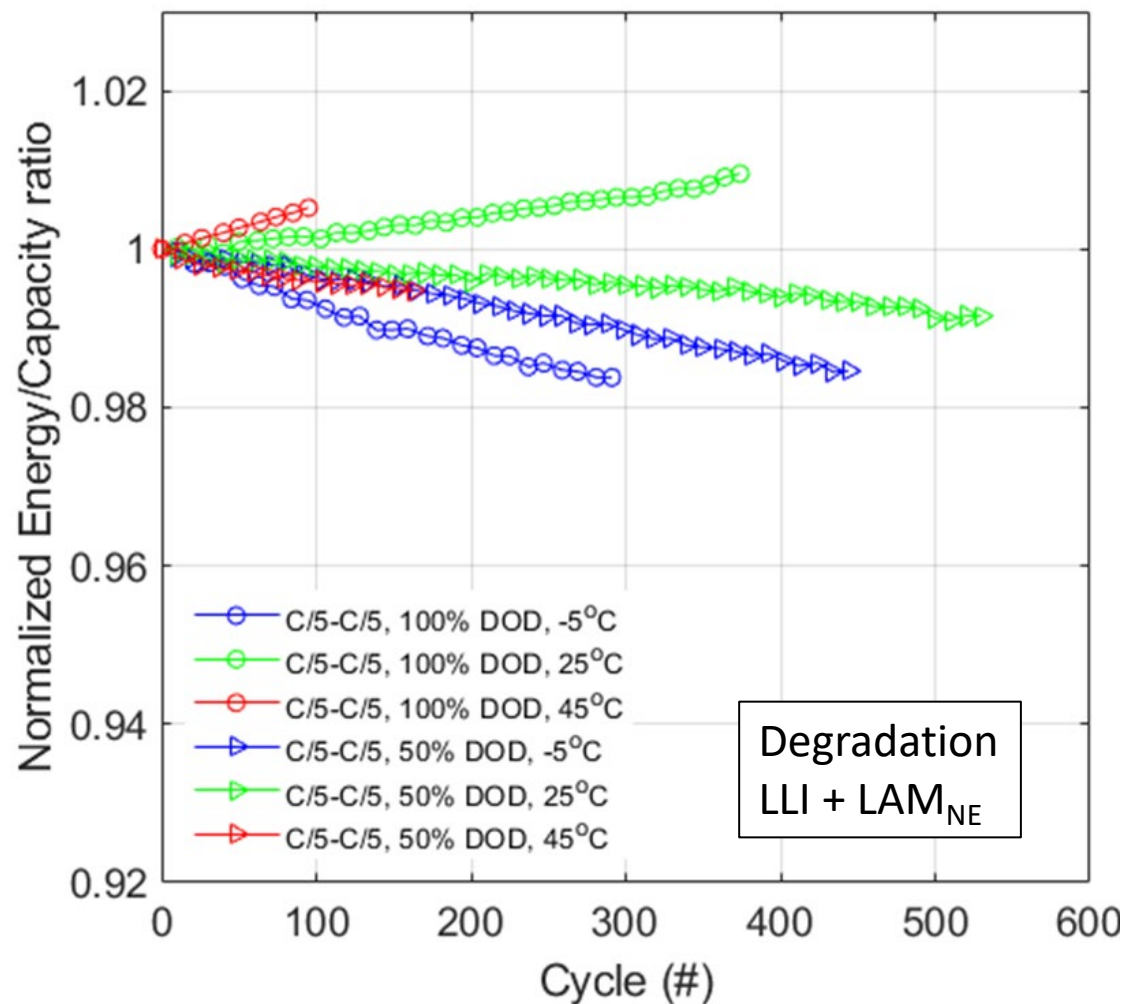
NMC<sub>111</sub>, Emulation of the full-cell response from half-cell data @ C/5



# Relating Capacity and Energy Losses

## Individual Electrode Performance

NMC<sub>111</sub>, Emulation of the full-cell response from half-cell data



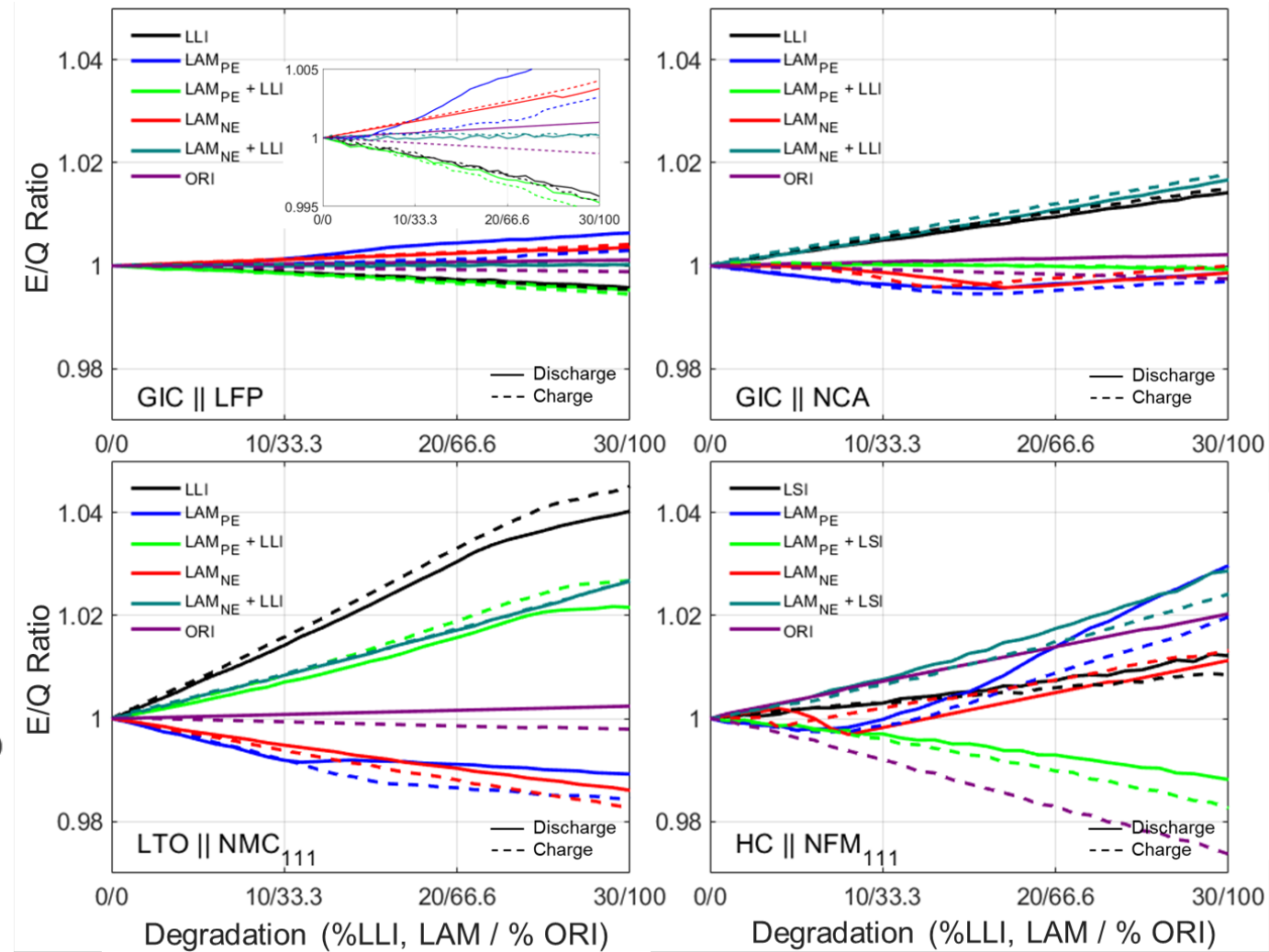
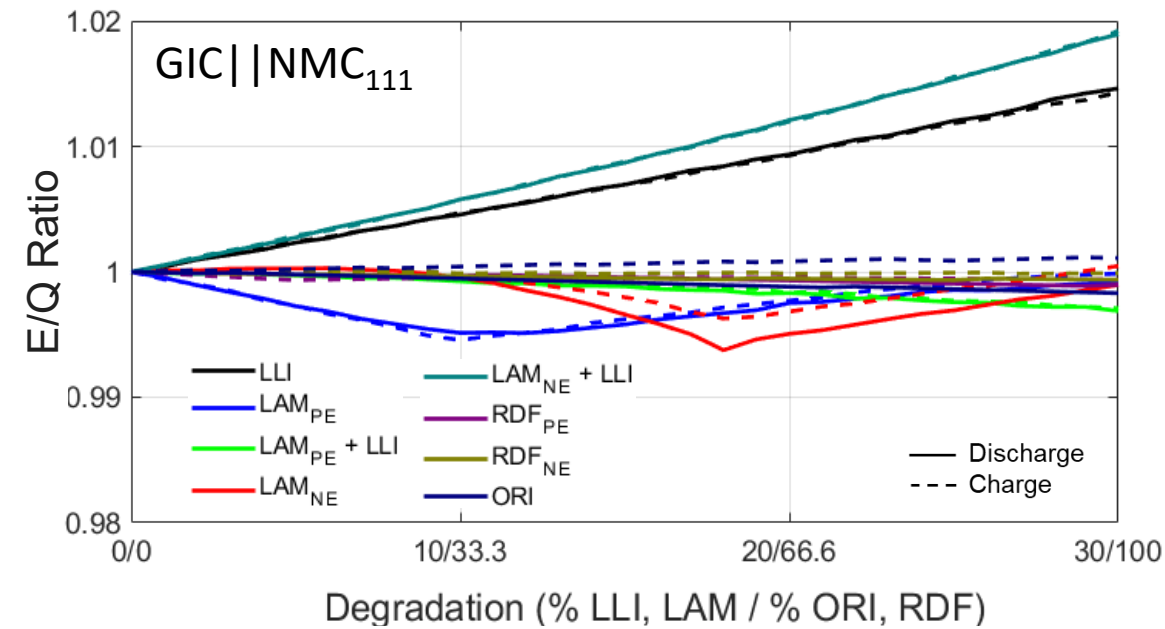
# Relating Capacity and Energy Losses

## Individual Electrode Performance

Can it be generalized to other chemistries?

Yes for NCA and  $\text{NMC}_{811}$

No for LFP, LTO, or Na-ion based cells



# Relating Capacity and Energy Losses

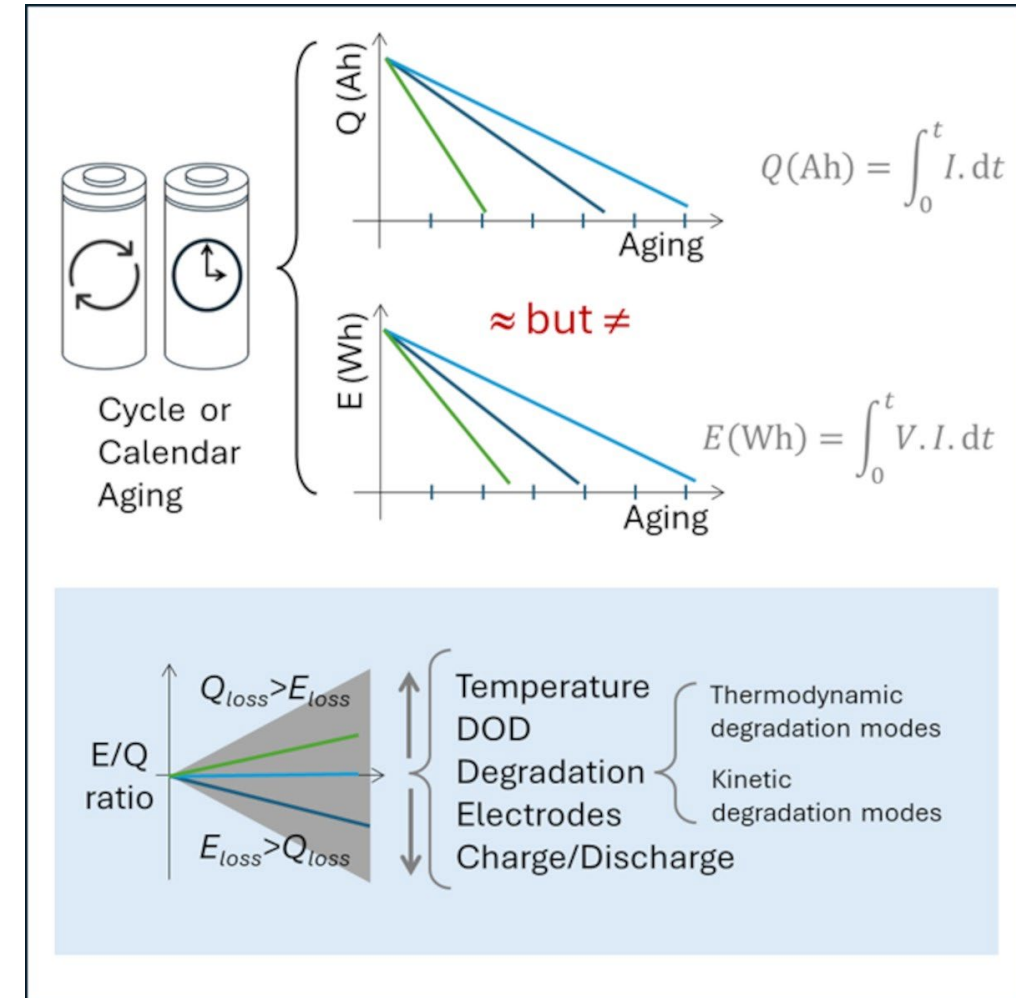
## Conclusions

This work defined and validated a mechanistic framework for the evolution of the energy-to-capacity ratio:

- Highly sensitive to the cell degradation path.
- Evolution not straightforward
  - Net result of multiple competing factors.
- Impact of each degradation mode is also chemistry dependent.
  - LLI increased along ratio layered oxides but decreased for LFP
  - RUL underestimation for layered oxides, overestimation for LFP**
- Predominantly dominated by kinetics at higher rates
- Strongly DOD dependent.

Tracking the E/Q ratio alongside capacity measurements appears crucial for more accurate monitoring and management across the battery lifecycle.

In addition, it might also better reflect the cell power fade than the resistance variations because it encompasses both thermodynamic and kinetic components.



# Acknowledgments

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*Thank you!*

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