



Multi-scale Thermal Stability of Lithium-Ion Batteries as a Function of Chemistry and State of Charge

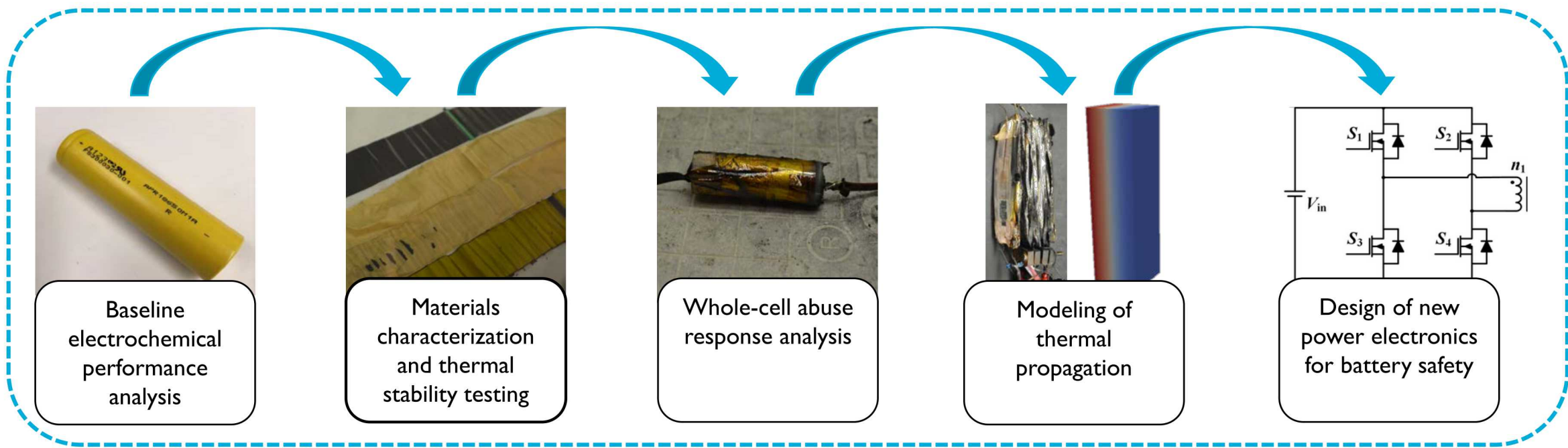
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Motivation & Objectives

Experimentally quantify Li-ion battery failure at the materials level during abusive and non-abusive conditions to enable:

- ...informed decision making about preferred operating conditions for different batteries
- ...modeling of battery degradation and thermal propagation
- ...translation of failure understanding to technologies for intervention
- ...safe and reliable energy storage for a resilient grid

- Relate component to whole cell failure for popular commercial Li-ion chemistries
- Compare failure response from fully charged to fully discharged state

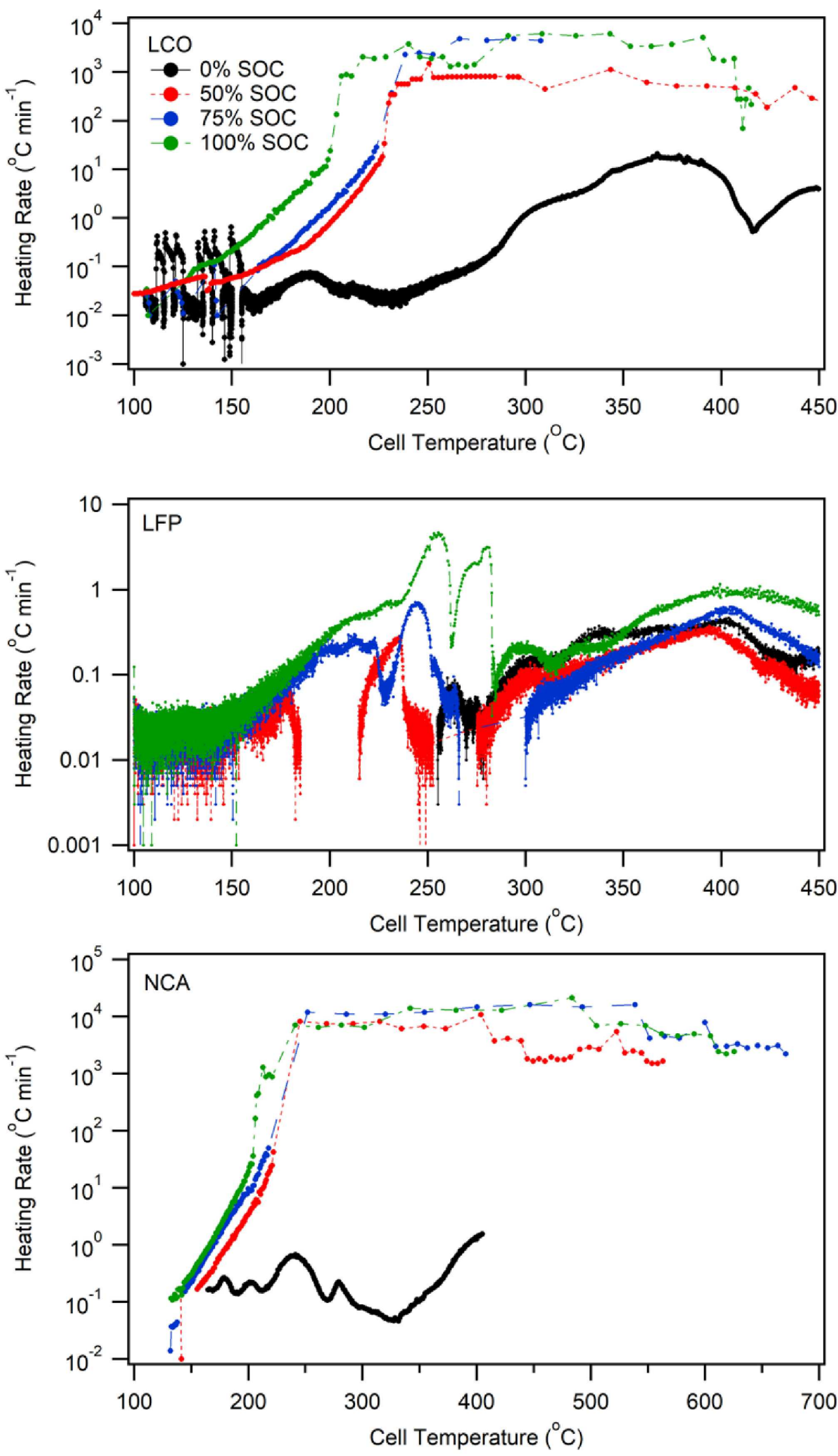


Milestones

- Whole cell calorimetry for LCO, LFP, NCA at 0, 50, 75, and 100% SOC
- Calorimetry of separator, anode, and cathode components at 0, 50, 75, and 100% SOC

Whole Cell Failure

Accelerating rate calorimetry (ARC) of 18650 Li-ion cells

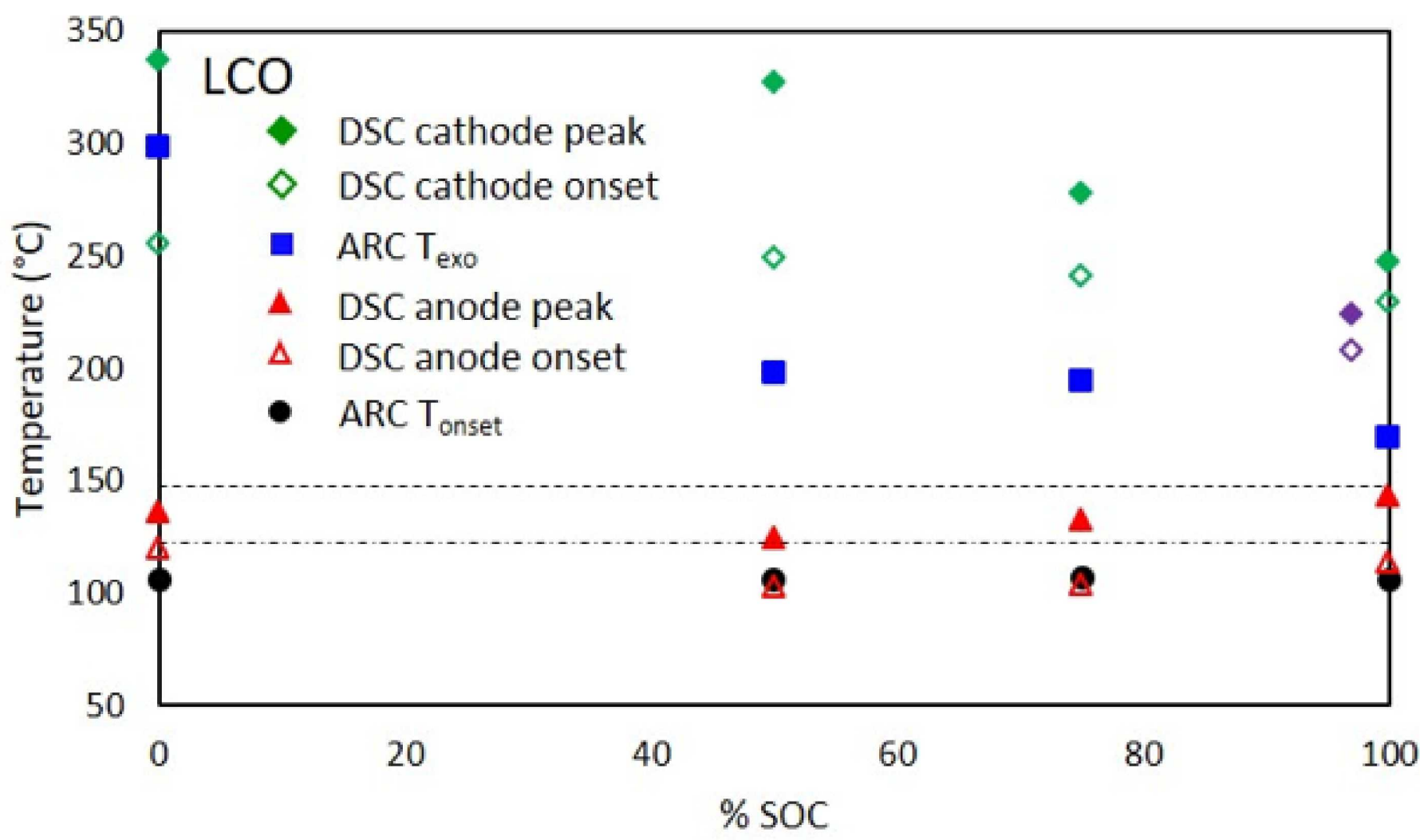


Cell	SOC (%)	T _{onset} (°C)	T _{exo} (°C)	HR _{max} (°C min ⁻¹)	HR _{max,norm} (°C min ⁻¹ Ah ⁻¹)
LCO	0	105.8	298.1	18.4	7.4
	50	96.6	202.5	1116.9	447
	75	106.5	193.3	4822.3	1930
	100	106.4	168.4	6053.5	2420
LFP	0	105.9	---	0.4	0.4
	50	100.8	---	0.3	0.3
	75	100.7	---	0.7	0.6
	100	100.9	240.5	4.5	4.1
NCA	0	164.9	391.8	1.5	0.5
	50	140.7	182.2	10810.3	3730
	75	131.7	169.4	16107.4	5550
	100	132.5	165.9	21480.4	7410

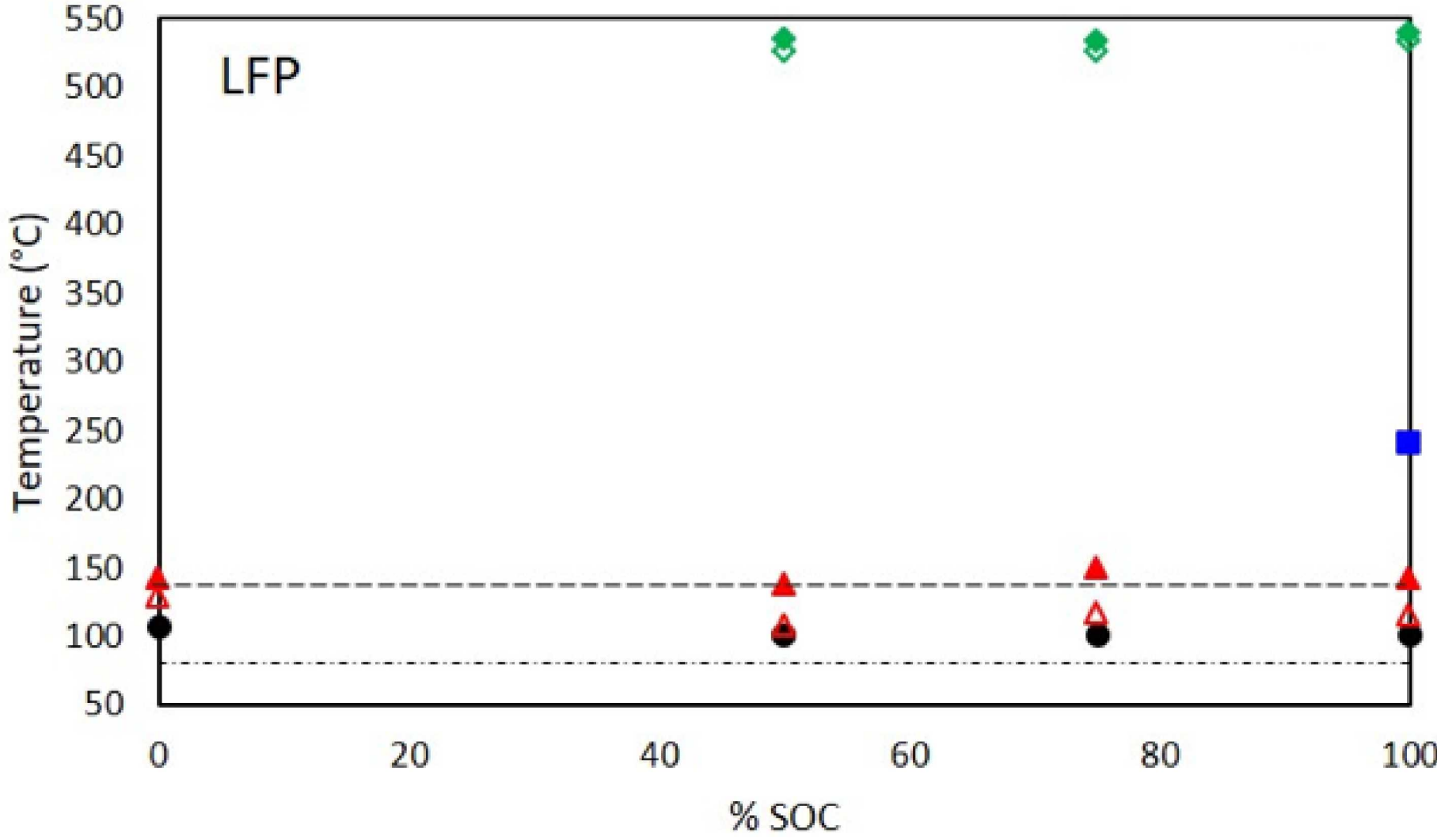
T_{onset}: self-heating (> 0.02 °C min⁻¹); T_{exo}: thermal runaway (> 1 °C min⁻¹)

Multi-scale Comparison

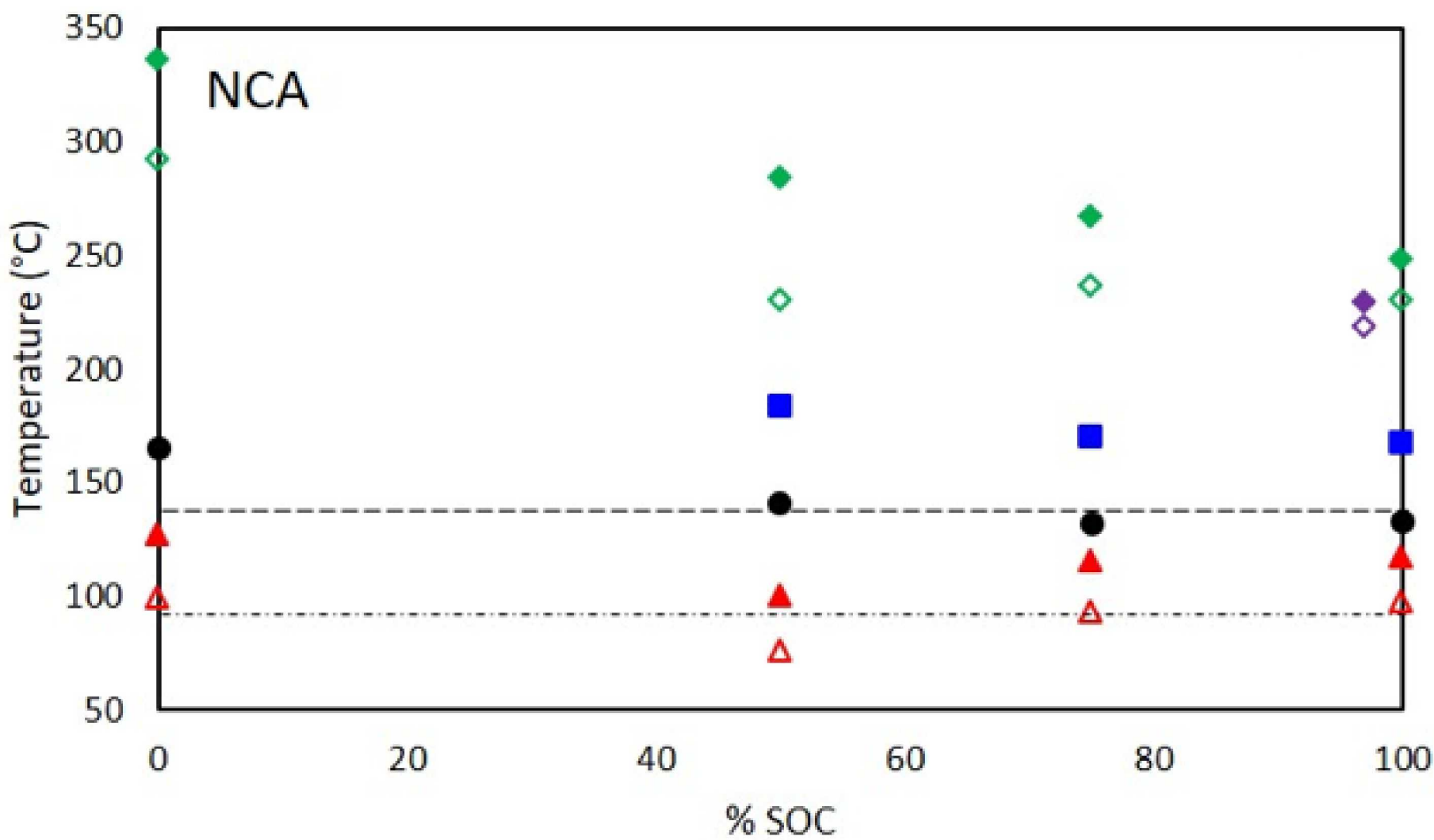
Metal oxide cathodes contribute to runaway only in combination with solvent



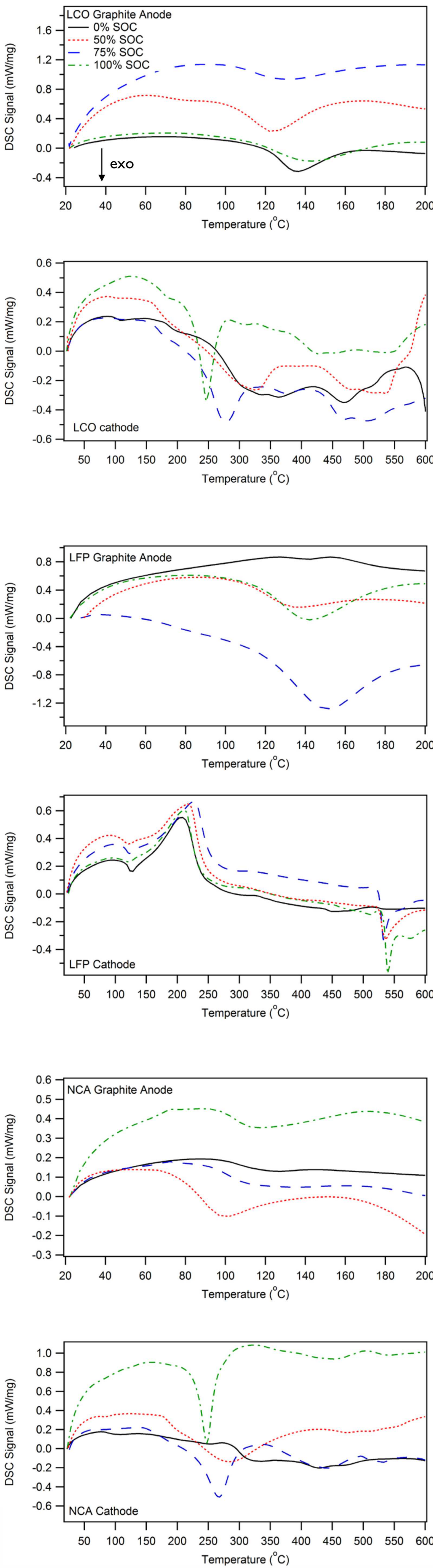
LFP cathode does not contribute to thermal runaway



Runaway onset not always coinciding with anode onset exotherm



Differential scanning calorimetry (DSC)



Conclusions

- Variability in key ARC temperatures can be traced back to cell component chemistry and SOC
- SEI decomposition is typically the onset of thermal runaway and does not vary with SOC
- LFP cathode does not contribute to runaway; metal oxides contribute only in combination with solvent
- Importance of standard calorimetry protocols to get 'true' onset temperatures

Publications: Barkholtz et al. *J. Power Sources* **2019**, 435, 226777
Shurtz et al. *J. Electrochem. Soc.* **2019**, 166, 12, A2498-A2502.

Presentations: 2019 Electrochemical Society Spring Meeting
Other: Development of nation-wide calorimetry collaborative