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Challenging Common Assumptions About Solid-State Battery Safety

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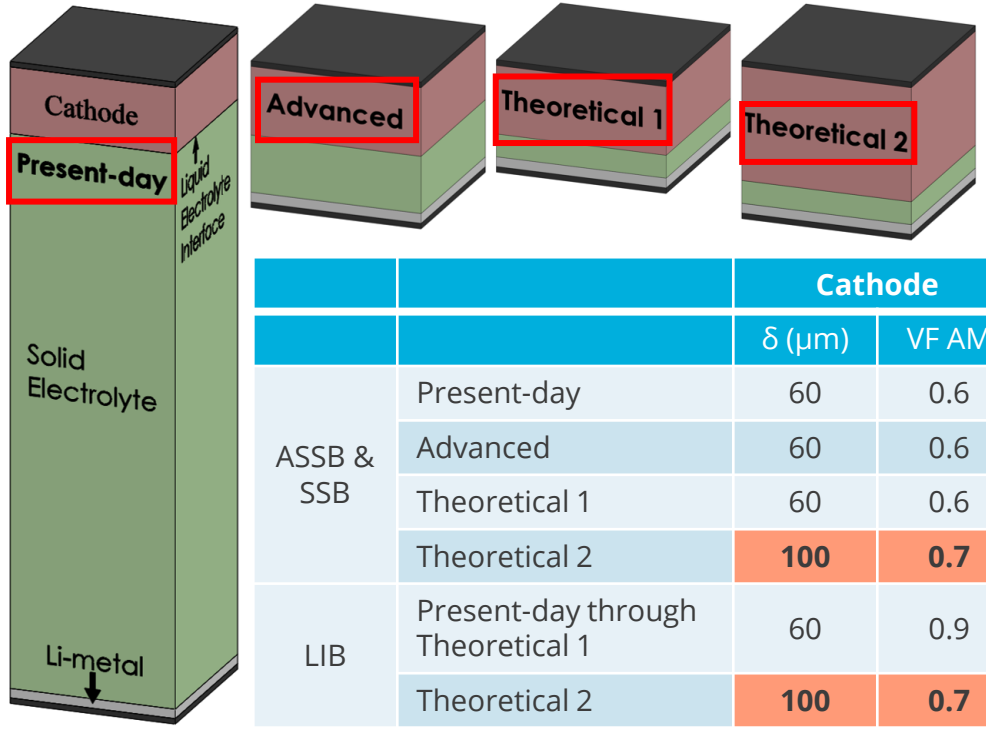
Summary

Motivation

- Solid-state electrolytes are believed to enhance safety
  - Interfacial resistance remains a key challenge
- Liquid electrolyte has been shown to reduce interfacial resistance
  - A question arises regarding the safety impact of liquid electrolyte inclusion
- Thermal modeling utilized to explore the safety impact of liquid electrolyte

Key Findings

- A small enough amount of liquid electrolyte has little effect on heat release
- Separator failure and specific heat release may be more consequential than the addition of liquid electrolyte
- External heating failure does not necessarily result in cascading propagation



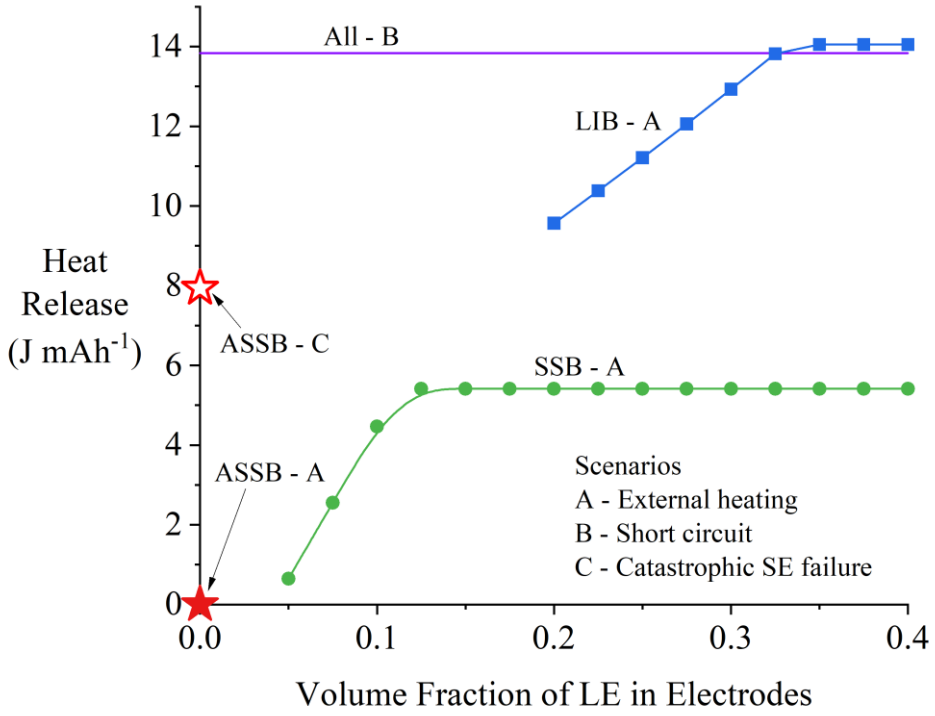
Cathode - NMC111
SE - LLZO
Liquid Electrolyte - $LiPF_6$ in EMC
Anode – Graphite or Li-metal

		Cathode		SE/Separator
		δ (μm)	VF AM	δ (μm)
ASSB & SSB	Present-day	60	0.6	**500**
	Advanced	60	0.6	**50**
	Theoretical 1	60	0.6	**20**
	Theoretical 2	**100**	**0.7**	20
LIB	Present-day through Theoretical 1	60	0.9	20
	Theoretical 2	**100**	**0.7**	20

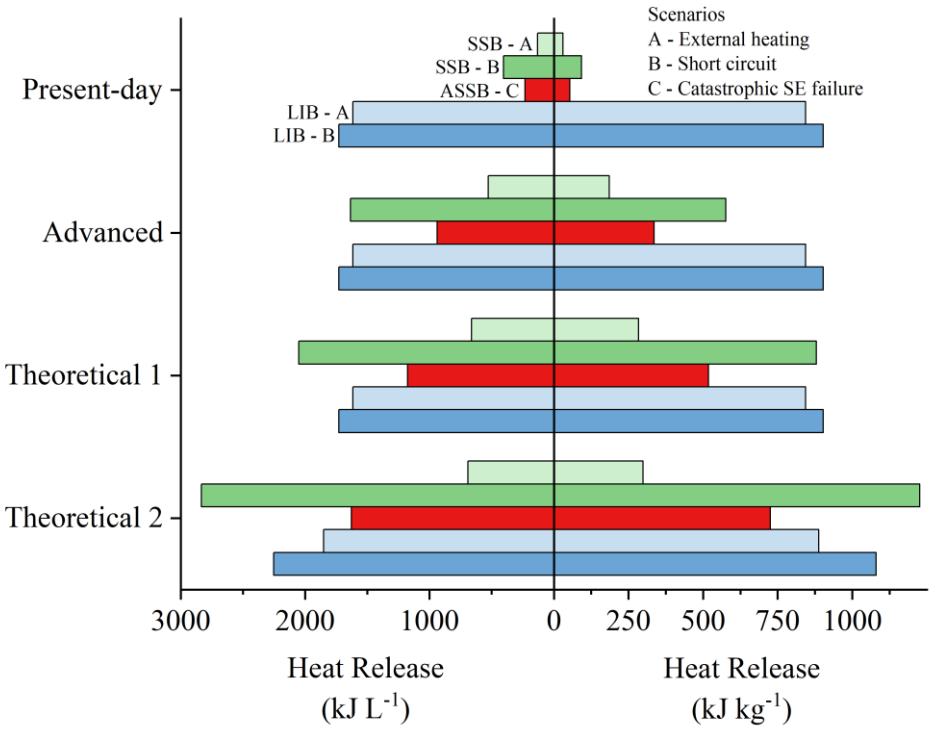
Thermal Model Scenarios and Heat Release as a Function of Liquid Volume Fraction

Scenario	Failure Mode	Key Assumptions
A	**External heating**	No SE/separator failure, SE is non-permeable
B	**Short circuit**	Other forms of heat release are zero
C	**Mechanical failure**	Only applied to ASSB

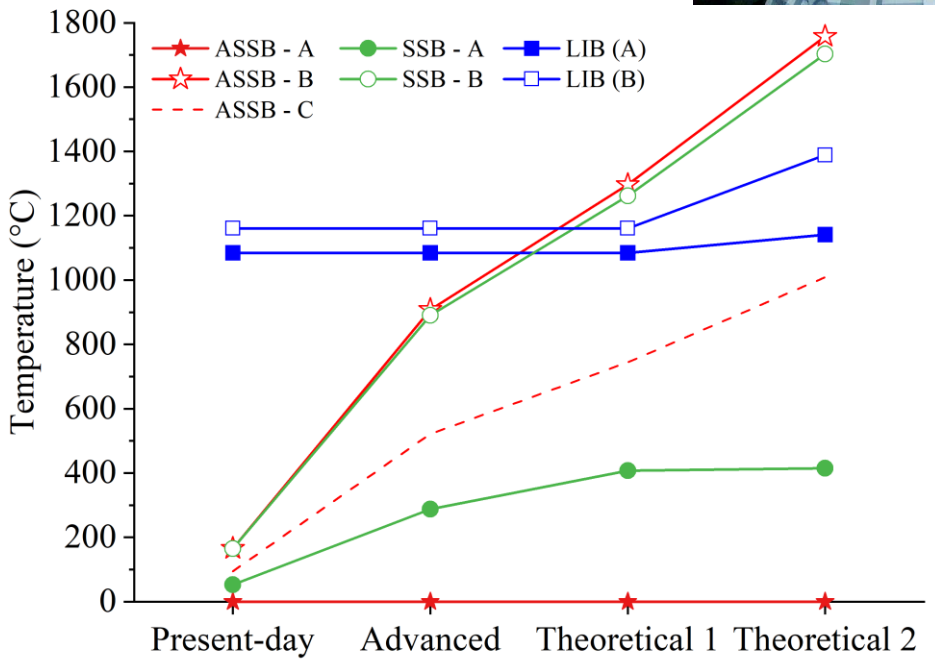
- LIB heat release is nearly double that of SSB
- SE failure in the ASSB allows O_2 to react with Li, releasing substantial heat
- A small enough amount of liquid electrolyte has little effect on heat release



Heat Release Dependance on Cell Format and Potential Temperature Rise



- SSB heat release due to external heating surpasses LIB when the SE is 20 μm thick
- Separator failure is more consequential than the addition of liquid electrolyte
- Specific heat release will become an important issue



- ASSB and SSB potential temperature rise due to short circuit surpasses LIB
- SE failure in the ASSB results in potential temperature rise rivaling the LIB
- External heating failure does not necessarily result in cascading propagation

Conclusions

- A compromise may be possible between cost, manufacturability, performance, and safety risk by varying the amount of liquid electrolyte
- As energy density is improved, separator failure and specific heat release becomes more consequential
- Certain failure modes may not result in cascading propagation even with liquid electrolyte inclusion

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Co-Authors

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Presentations

- A. Bates, "Overcharge Tolerance of LiFePO4 Cathode Pouch Cells", 240th ECS Meeting, Virtual, October 10-14, 2021.
- A. Bates, "Thermal Modeling of Liquid Electrolyte in Solid-State Batteries", Solid-State Battery Summit, Virtual, August 3-4, 2021.

Publications

- A. Bates, J. Langendorf, C. Grosso, J. Lamb, S. Ivanov, L. Jauregui, J. Kustas, Y. Preger, L. Torres-Castro, "Degradation and Structural Changes of LiFePO4 Cathodes of Li-ion Batteries Exposed to Overcharge Conditions", Journal of the Electrochemical Society. (In Preparation)
- A. Bates, Y. Preger, L. Torres-Castro, K.L. Harrison, S.J. Harris, J. Hewson, "Safety Impacts of Liquid Electrolyte Inclusion in Solid State Batteries", Joule. (Submitted)
- L. Torres-Castro, Y. Preger, A. M. Bates, J. McDowall, M. Abreu-Sepulveda "Lithium-Ion Batteries" chapter submitted in Cambridge Elements, Grid Energy Storage.

Other

- A. Bates, Lead Organizer MRS Symposium, "Practical Challenges Facing Solid-State Batteries: Performance, Safety, and Manufacturing", Committee Members: D. Buchberger, H. Zhu, and Y. Qi, MRS Fall Meeting, November 27 – December 2, 2022, Boston, Massachusetts.

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