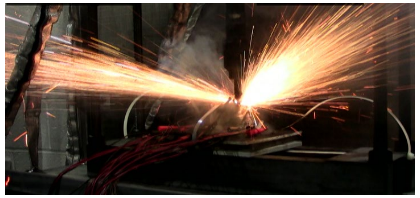
Funded by the U.S. Department of Energy, Office of Electricity, Energy Storage program under the guidance of Dr. Imre Gyuk, Program Director.

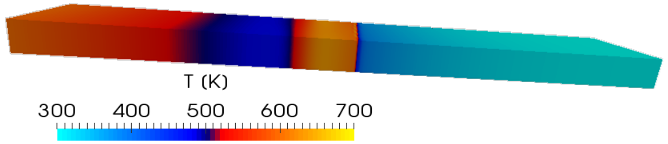
Explore the web calculator:

https://www.sandia.gov/ess-ssl/thermodynamic-web-calculator/about.html

Sandia National Laboratories

# A Lithium-Ion Battery Thermodynamic Web Calculator for Thermal Runaway Severity Assessments






PRESENTED BY

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**DOE Office of Electricity Energy Storage Program Peer Review**

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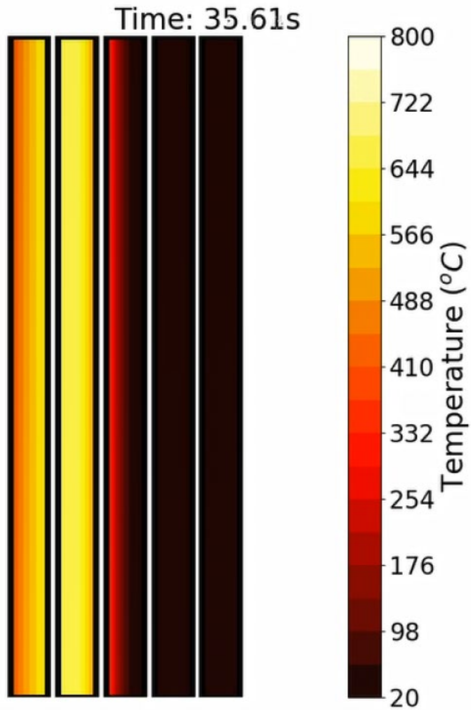
SAND2021-12929 PE

# Why do Batteries Have a Risk of Thermal Runaway?

- Rapid release of stored energy in any form is hazardous
  - Thermal, mechanical, pressure, chemical, or potential energy
  - Stored energy must have an unstable aspect to be accessible
- Undesired reactions may activate under certain conditions for stored chemical energy (batteries and fuels)
  - Li-ion battery electrodes decompose at high temperatures
    - External heating or internal shorts provide sufficient ignition energy
    - Energy from decomposition may exceed stored electrical energy
    - A single cell may ignite cascading thermal runaway in neighbors

Catastrophic failure of Teton Dam on June 5, 1976, ID-L-0010, WaterArchives.org




www.cnn.com

# How Much Heat Can Be Released If My Li-Ion Battery Goes Into Thermal Runaway?

- Simple or complex safety assessments require **quantity of heat released**
  - Requires thermodynamic properties that can be hard to find
  - Simple assessments need total potential heat release
  - Advanced thermal runaway models need heat for each decomposition reaction
- **Solution from Sandia**: Lithium-Ion Battery Thermodynamic Web Calculator
  - https://www.sandia.gov/ess-ssl/thermodynamic-web-calculator/
  - Predicts potential heat release from user-defined cathodes and full cells
  - Customizable cathode composition, state of charge, and cell build/size
- Video demo on next slide

# Lithium-ion Battery Thermodynamic Web Calculator

This web-based calculator estimates heats of reaction associated with thermal runway of layered metal oxide cathode materials based on the underlying thermodynamics for specific metal compositions, degrees of delithiation, and coexisting organic material (e.g. electrolyte solvent).

The web-based calculator is intended to provide a better experience for most users, while the spreadsheet-based calculator is suitable for customization by advanced users.

Enter Thermodynamic Web Calculator

Download Thermodynamic Excel Calculator

If you use this calculator to support analysis that is submitted for publication in any form, **please cite this website and the articles listed below.**

These thermodynamic calculations are explained in the following articles:

R. C. Shurtz and J. C. Hewson, *J. Electrochem. Soc.*, 2020, 167, 090543

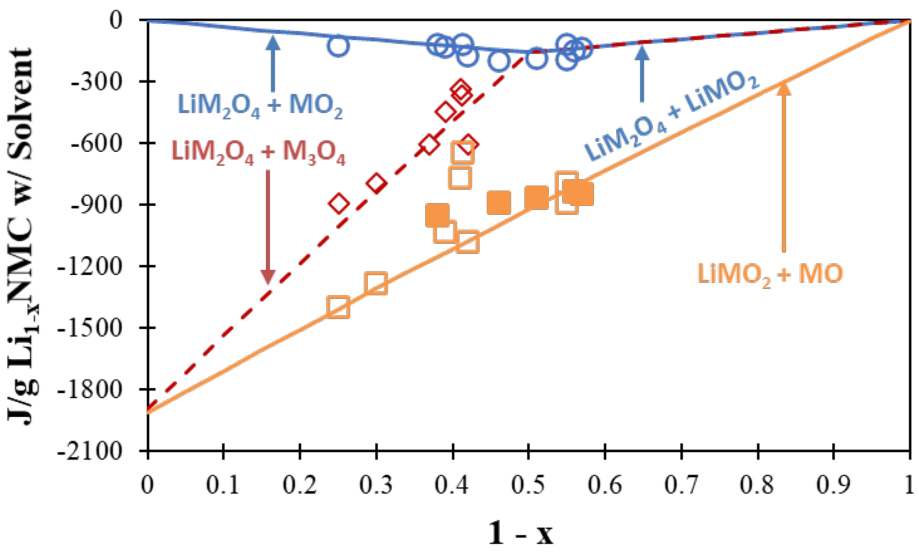
R. C. Shurtz, *J. Electrochem. Soc.*, 2020, 167, 140544

The proper citation for this website is:

Shurtz, Randy C. (2021) "Lithium-ion Battery Thermodynamic Web Calculator," Sandia National Laboratories, https://www.sandia.gov/ess-ssl/thermodynamic-web-calculator/

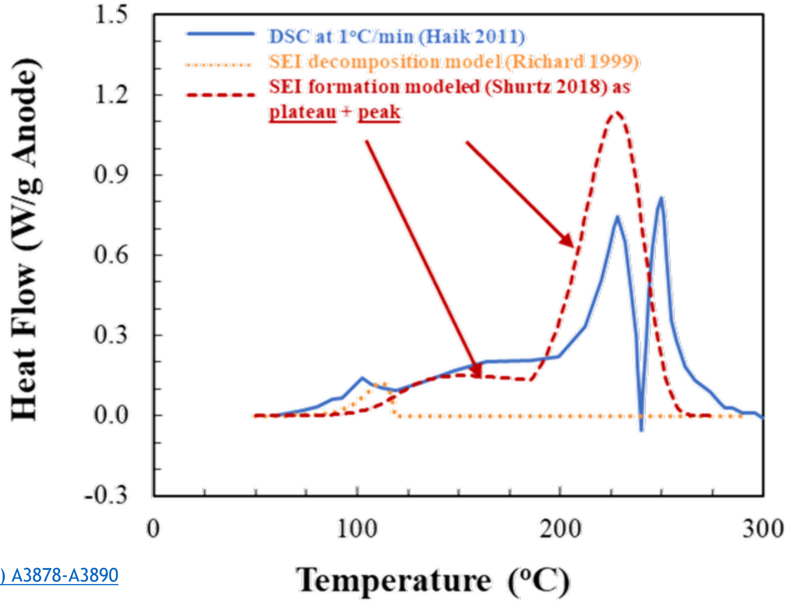
# Source and Performance of Thermodynamic Web Calculations

- Thermodynamic properties and reaction definitions from recent review[1]
- Methods compare favorably with thermal measurements
  - Layered metal oxide positive electrode[2] with arbitrary mix of Ni, Mn, Co, and/or Al
  - Graphite negative electrode[3]
  - Common electrolyte solvents, any state of charge
- Future updates to include more electrode materials and improved user interface
  - Contact for suggested improvements: libtrwebcalc@sandia.gov
- Thermal runaway models at Sandia couple measured decomposition rates with predicted stepwise heats of reaction from this tool




Thermodynamic Cathode Heat Release Comparison[2]

Graphite Heat Release Comparison[3]





1. R. C. Shurtz and J. C. Hewson, *J. Electrochem. Soc.*, 2020, 167, 090543
2. R. C. Shurtz, *J. Electrochem. Soc.*, 2020, 167, 140544
3. Shurtz, R. C., J. D. Engerer and J. C. Hewson, *J. Electrochem. Soc.*, 2018, 165(16) A3878-A3890