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Data Article

Dataset of mechanically induced thermal runaway measurement and severity level on Li-ion batteries



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ABSTRACT

The deployment of Li-ion batteries covers a wide range of energy storage applications, from mobile phones, e-bikes, electric vehicles (EV) to stationary energy storage systems. However, safety issue such as thermal runaway is always one of the most important concerns preventing Li-ion batteries from further market penetration. A standardized single-side indentation test protocol was developed to mechanically induce an internal short-circuit. The cell voltage, compressive load, indenter stroke, and temperature at the indentation point are measured in time series. The test data of each cell, along with cell parameters such as dimensions, mass, chemistry, state of charge (SOC), capacity, are integrated to calculate a thermal runaway severity score from 0 to100. Complete data collection process including the original measured record, test method, severity score calculation scheme is presented in this article. The thermal runaway severity analysis and the more than 100 tested Li-ion battery records provide a good

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data source for further comparison and ranking of thermal runaway risks.

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Specifications Table

Subject	Energy, Energy Engineering and Power Technology Business, Management and decision sciences/Safety, Risk, Reliability and Quality
Specific subject area	Use standardized single-side indentation test data to categorize the thermal runaway risk of Li-ion batteries.
Data format	Raw, Analyzed
Type of data	Table, Chart
Data collection	The test system consists of a load frame that moves down the indenter to apply compressive load on Li-ion battery. A load cell is used to measure the compressive force applied to the cell. The voltage and temperature of the cell near the indentation location (by using thermalcouple) are collected by LabViewTM program. An infrared camera is used to monitor cell surface temperature. The thermal runaway severity level is calculated by the recorded voltage signal and temperature history throughout the test.
Data source location	Sandia National Laboratories and Oak Ridge National Laboratory.
Data accessibility	Repository name: Mechanically Induced Thermal Runaway for Li-ion Batteries Data identification number: 10.17632/sn2kv34r4h.1
	Direct URL to data: www.batteryarchive.org,
	https://data.mendeley.com/datasets/sn2kv34r4h/1.
	Instructions for accessing these data: All data can be anonymously accessed by the public. The BatteryArchive is supported by the U.S. Department of Energy Office of Electricity Energy Storage Program through the Sandia National Laboratories Grid Energy Storage Department.
Related research article	Lin, Lianshan, et al. "Mechanically induced thermal runaway severity analysis for Li-ion batteries." Journal of Energy Storage 61 (2023): 106798.
	https://doi.org/10.1016/j.est.2023.106798

1. Value of the Data

- These data provide comprehensive and standardized single-side indentation test results on Li-ion cells in different chemistries, capacities and SOCs.
- The dataset also includes a calculated thermal runaway severity score for each cell which is compatible with different types of Li-ion batteries with various SOCs, chemistries, and capacities.
- The raw tested data, along with the analyzed data, will provide battery designers, manufacturers, and end-users a clear comparison of thermal runaway severity of different batteries.
- These data can be reused by other researchers to develop their own battery thermal runaway evaluation criteria.
- The thermal runaway severity evaluated through the single-side indentation method in this article applies best to Li-ion cells in mechanical abuse condition.

2. Background

The pursuit of batteries with higher power density and lower cost often introduces new safety and reliability challenges. Safety hazards of Li-ion batteries have been well-documented and thermal runaway has been identified as a critical concern in the deployment of the technology. How to evaluate and grade the thermal runaway severity of Li-ion batteries in a safe experimental environment has gradually drawn broad interest in the battery community. The

single-side indentation test provides comprehensive and standardized results on Li-ion cells in different chemistries, capacities and SOCs. Sharing the raw tested data, along with the analyzed data through this article will provide battery designers, manufacturers, and end-users a comprehensive understanding of thermal runaway severity of different batteries we have analyzed in our previous published article.

3. Data Description

The mechanically induced thermal runaway test dataset [1] in this article includes two parts, (a) the cell meta-data including the cell/test ID, capacity, SOC, observed severity level and analyzed thermal runaway score; (b) the measurements in the single-side indentation test, majorly consist of the time, cell voltage and temperature columns. The dataset in part (a) is stored in an excel file (e.g. main.xlsx) that has two worksheets ("Sheet1" and "Summary"). Data columns in these two worksheets are illustrated in Figs. 1 and 2. In general, worksheet "Sheet1" is used for data input, while the "Summary" worksheet lists the calculated thermal runaway score (Column D in Fig. 2) along with the input information and observed severity level (Column B and C in Fig. 2).

Under the same directory that main.xlsx is located, there is a subfolder "excel" that stores all the raw data files (.xlsx files) recording the voltage and temperature history in the indentation test, which includes all the part (b) dataset. Each data file in "excel" subfolder has file name agrees with the cell ID shown in Fig. 1 column A, or FileName column (column A) in "Summary" worksheet in Fig. 2. Taking the data file "Sorteria-100SOC-cell1.xlsx" as an example (Fig. 3), columns A and C stores the measured history data of time and corresponding cell volt-

	Cell/Test ID	Analyze St	atus Observed Severity Level	Capacity	SOC
4	A	ВС	D E	F	G
1	Sorteria-100SOC-cell1	Completed	No effect, instant local Joule heating, no internal discharge – 1	4960	100
2	Sorteria-100SOC-cell2	Completed	No effect, instant local Joule heating, no internal discharge – 1	4960	100
3	Sorteria-Control-100SOC-cell1	Completed	Physical effect, rupture of pouch, smoke, gas release, fire - 7	5190	100
4	Sorteria-Control-100SOC-cell2	Completed	Physical effect, rupture of pouch, smoke, gas release, fire - 7	5190	100
5	LCO-LP-6400mAh-100SOC-cell1	Completed	Physical effect, rupture of pouch, smoke, gas release, fire – 7	6400	100
6	LCO-LP-6400mAh-100SOC-cell2	Completed	Physical effect, rupture of pouch, smoke, gas release, fire - 7	6400	100
7	LCO-LP-6400mAh-80SOC-Cell3	Completed	Physical effect, rupture of pouch, smoke, gas release, fire - 7	6400	80
8	LCO-LP6400mAh-80SOC-cell4	Completed	Physical effect, rupture of pouch, smoke, gas release, fire - 7	6400	80
9	Soetria-80SOC-cell3	Completed	Physical effect, rupture of pouch, smoke, gas release, fire - 7	4960	80
10	Sorteria-Control-60SOC-cell1	Completed	Physical effect, rupture of pouch, smoke, gas release, fire - 7	5190	60
11	Soetria-Control-45SOC-cell1	Completed	Physical effect (pouch swelling), rupture of pouch, gas release - 6	5190	45
12	Sorteria-control-40SOC-cell2	Completed	Physical effect (pouch swelling), rupture of pouch, gas release - 6	5190	40
13	Sorteria-control-20SOC-cell1	Completed	Physical effect (pouch swelling), extended joule heating, local reactions – 5	5190	20
14	Soteria-control-30SOC-cell2	Completed	Physical effect (pouch swelling), extended joule heating, local reactions – 5	5190	30
15	Soteria-control-30SOC-cell1	Completed	Physical effect (pouch swelling), extended joule heating, local reactions – 5	5190	30

Fig. 1. Data columns of Sheet1 worksheet in main.xlsx.

4	A	В	C	D	E	F
1	FileName	Observed Severity Level	Observed Score	Calculated Score	Capacity	SOC
2	Sorteria-100SOC-cell1	No effect, instant local Joule heating, no internal discharge – 1	1.00	5.00	4960	100
3	Sorteria-100SOC-cell2	No effect, instant local Joule heating, no internal discharge - 1	1.00	5.00	4960	100
4	Sorteria-Control-100SOC-cell1	Physical effect, rupture of pouch, smoke, gas release, fire - 7	7.00	100.00	5190	100
5	Sorteria-Control-100SOC-cell2	Physical effect, rupture of pouch, smoke, gas release, fire - 7	7.00	100.00	5190	100
6	LCO-LP-6400mAh-100SOC-cell1	Physical effect, rupture of pouch, smoke, gas release, fire - 7	7.00	100.00	6400	100
7	LCO-LP-6400mAh-100SOC-cell2	Physical effect, rupture of pouch, smoke, gas release, fire - 7	7.00	100.00	6400	100
8	LCO-LP-6400mAh-80SOC-Cell3	Physical effect, rupture of pouch, smoke, gas release, fire - 7	7.00	100.00	6400	80
9	LCO-LP6400mAh-80SOC-cell4	Physical effect, rupture of pouch, smoke, gas release, fire - 7	7.00	97.48	6400	80
10	Soetria-80SOC-cell3	Physical effect, rupture of pouch, smoke, gas release, fire - 7	7.00	100.00	4960	80
11	Sorteria-Control-60SOC-cell1	Physical effect, rupture of pouch, smoke, gas release, fire - 7	7.00	100.00	5190	60
12	Soetria-Control-45SOC-cell1	Physical effect (pouch swelling), rupture of pouch, gas release - 6	6.00	60.73	5190	45
13	Sorteria-control-40SOC-cell2	Physical effect (pouch swelling), rupture of pouch, gas release - 6	6.00	57.93	5190	40
14	Sorteria-control-20SOC-cell1	Physical effect (pouch swelling), extended joule heating, local reactions - 5	5.00	40.28	5190	20
15	Soteria-control-30SOC-cell2	Physical effect (pouch swelling), extended joule heating, local reactions – 5	5.00	55.53	5190	30

Fig. 2. Data columns of Summary worksheet in main.xlsx.

4	A	В	C	D	Ε	F	G	н	1	T	U	V	W	X
1	Time (second)	Load (lb)	Voltage (V)	Encoder (in)		Time (sec)	Penetrator Force (N)	Cell Voltage (V)	Displacement (mm)	Time (sec)	TC1 (°C)	TC2 (°C)	TC3 (°C)	TC4 (°C)
2	0	-4.09	4.175	0		0	18.193	4.175	0	0	2.12E+01			
3	0.124	-3.809	4.175	0		0.124	16.943	4.175	0	0.099	2.12E+01			
4	0.219	-4.105	4.173	0		0.219	18.260	4.173	0	0.2	2.12E+01			
5	0.372	-4.141	4.173	0		0.372	18.420	4.173	C	0.3	2.12E+01			
6	0.428	-4.017	4.173	0		0.428	17.868	4.173	0	0.4	2.12E+01			
7	0.693	-4.06	4.173	0		0.693	18.060	4.173	C	0.501	2.12E+01			
8	0.744	-3.757	4.173	0		0.744	16.712	4.173	0	0.6	2.12E+01			
9	1.043	-4.049	4.173	0		1.043	18.011	4.173	0	0.702	2.12E+01			
10	1.157	-4.484	4.173	0		1.157	19.946	4.173	0	0.801	2.12E+01			
11	1.283	-4.119	4.173	0		1.283	18.322	4.173	0	0.935	2.12E+01			
12	1.418	-4.235	4.172	0		1.418	18.838	4.172	0	1.001	2.12E+01			
13	1.463	-3.848	4.174	0		1.463	17.117	4.174	0	1.101	2.12E+01			
14	1.568	-3.918	4.173	0		1.568	17.428	4.173	0	1.201	2.12E+01			
15	1.705	-4.089	4.173	0		1.705	18.189	4.173	0	1.3	2.12E+01			

Fig. 3. Data columns of Sheet1 worksheet in Sorteria-100SOC-cell1.xlsx.

age, columns T and U stores the temperature history measured from thermocouple (or infrared camera) nearby the contact point between the indenter and cell. Column B in Fig. 3 records the load signal from load cell, which is in pound (lb). Column D in Fig. 3 stores the original encoder stroke in inches. For calculation convenience, the loading force is transferred into Newtons in column G, the encoder is transferred into displacement in mm in column I, and column F is the corresponding time history that repeats value in column A. In some tests, more thermocouples or infrared sensors are assigned to the test cell. In this case, additional columns such as V, W and X in Fig. 3 are prepared for storing more temperature data. Though data files tested in different organizations might have these temperature, voltage, displacement and force data stored in different columns, their column titles with the corresponding units included can help identify the measured physical variables. All the data files in "excel" subfolder share the same data structure and formatting, which provides consistency and conveniency of analyzing the thermal runaway severity score in main.xlsx.

The data from the mechanical indentation experiments have also been uploaded to Battery Archive, the first public repository for visualization, analysis, and comparison of battery data across institutions. [2,3] Here, mechanical indentation results from all experiments and institutions have been imported into a common format and searchable database. All experiments include metadata for the cell ID, anode, cathode, source, capacity, form factor, SOC, indenter diameter, and indenter speed. The full database may be filtered based on the testing institution and battery SOC. Once certain cells are selected, the site populates pre-set plots, including displacement, temperature, force, and voltage versus time. This automated plotting facilitates quick evaluation of the data prior to download and further analysis. Fig. 4 gives an example of the dashboards on the Battery Archive public site.

4. Experimental Design, Materials and Methods

The Oak Ridge National Laboratory (ORNL) and Sandia National Laboratories (Sandia) have developed a single-side mechanical indentation test illustrated in Fig. 5. The indenter was driven by electrical servo motor in ORNL test facility, while the Sandia one was driven by hydraulic system. Note that the temperature data might be recorded from the thermocouples shown in Fig. 5 (b), or be extracted from the thermal imaging system if an infrared camera is employed. The six thermocouples (TC1~TC6) illustrated in Fig. 5 (b) are attached either on the indentation side or back side of the cell to collect the temperature data through the test. If only one thermocouple is assigned, then TC1 is actually at the location of TC6 illustrated in the figure. The indentation test is similar to the blunt nail [4] test and the USABC small indentation test [5]. The international penetration test standards for the cells, such as SAE J2464, SAE J2929, ISO 12405-1 [6] provide some useful information to development of the indentation test in this work. Though different test facilities were developed, the indentation tests were performed at both laboratories by following the same test protocol listed in Table 1.

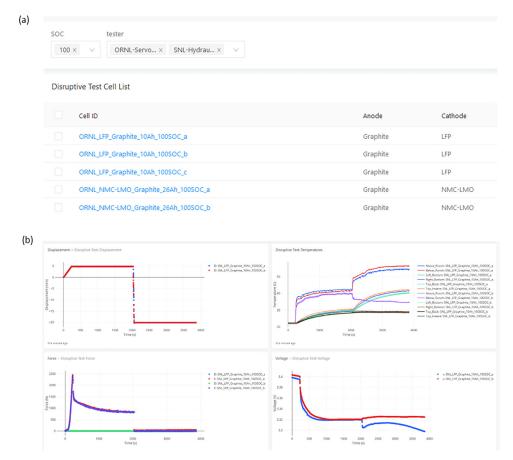


Fig. 4. Dashboards in the Battery Archive public site showing (a) a list of cells with metadata for filtering and (b) plots of force, displacement, voltage, and temperature versus time for two replicate cells. The 10 Ah cells have an LFP cathode, graphite anode, and underwent mechanical indentation testing at 100 % SOC. Automated plotting enables immediate assessment of the consistency of the experimental results.

The thermal runaway severity levels are used for initial assessment of cell indentation results. The severity levels defined in the EUCAR table [7] are observation-based cell response and function after the test. They do not have the sensitivity to distinguish cells with different chemistries, capacities, and SOCs. In this work, thermal runaway severity analysis is based solely on the recorded data in indentation tests. The calculated hazards severity (CHS) utilizes the collected temperature and voltage data to differentiate the hazards levels in different batteries. Note that the thermal runaway of Li-ion cells could be caused by either the self-induced failure when the cell is under standard use condition, or by the abuse condition such as mechanical abuse, electrical abuse, and thermal abuse in practical use [8,9]. The thermal runaway severity estimated from the single-side indentation method in this article fits with the mechanical abuse condition best. The following terms are defined before performing the CHS calculation.

1. Max Temperature ($T_{\rm max}$): defined by the maximum temperature the sensor (thermocouple or infrared imaging device) monitors during the test. Note that this temperature is measured in an open test environment rather than an adiabatic system, so its measurement relies on the available sensor and intended temperature range, which has minor difference to the maximum temperature of reactant under thermal runaway defined in reference [10].

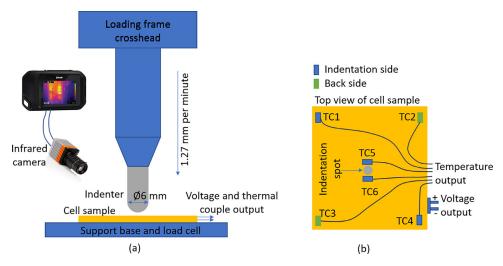


Fig. 5. Illustration of single-side indentation test (a) front view of test frame and cell sample; (b) top view of cell sample with thermocouples (TC1~TC6) attached.

Table 1Single-side indentation test protocols.

Test protocols		
Test sample		Single Li-ion pouch cell with capacity ranging from 0.5 Ahr up to 33 Ahr.
Indenter	Material and shape	Stainless steel sphere or blunt indenter presses on pouch center
	Diameter	6 mm for standard test and 12.7 mm for occasional comparison test.
	Cell support	Stainless steel block
Loading	Driver	Motor-driven or hydraulic loading system
	Speed	0.05 in. per minute (1.27 mm per minute)
Measurements/Monitoring	DAQ rate at 10 Hz or faster	Open circuit voltage Voc Load Displacement
	Cell surface temperature	Measured at locations next to the indenter, and multiple points on the surface, temperature on positive/negative tabs measured by thermocouples or IR imaging
Short-circuit Detection and		Voltage drop Voc >= 25 mV
Post-triggering Actions		Indenter stay in place for > 10 min
55 5		Keep recording Voc, Temperature, load and displacement for >5 min

- 2. Temperature Increase Rate (T_{\max}) : defined by the highest rate of temperature increase through the test, calculated by $(T_{i+1} T_i)/(t_{i+1} t_i)$ where T is temperature and t is time, i is the data series index.
- 3. Voltage Drop Score (V_{score}): an integer ranges from 1 to 5. Several voltage values are used in this score calculation, which are:
 - a) Initial Voltage V_{init} , the voltage value before running the test.
 - b) Voltage Range $V_{\rm range}$, the voltage difference between the peak value and the valley value through the test.

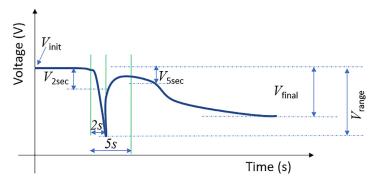


Fig. 6. illustration of voltage history and the definition of each voltage variables.

- c) Final Voltage Change $V_{\rm final}$, the voltage difference between the $V_{\rm init}$ and the value at the end of test that data collection stops and indenter moves back.
- d) Voltage Drop in 2 s V_{2sec} , the voltage difference between the peak value and the value at the next 2 s point.
- e) Voltage Drop in 5 s V_{5sec} , similar definition to the item d but only the drop is compared with the value at 5 s point.

The voltages illustrated in Fig. 6 help explain each definition. Determination of the V_{score} is defined below:

- If $(V_{\text{range}}/V_{\text{init}}) < 20 \%$, then $V_{\text{score}} = 1$, which indicates a very small voltage change through the test. This item fits with the situation that cell voltage has little drop through the test, so time is excluded in the calculation since it has insignificant impact on voltage change.
- If $(V_{\rm range}/V_{\rm init}) > 50$ % but the value $(V_{\rm final}/V_{\rm init}) < 20$ %, then $V_{\rm score} = 2$. In this case, the voltage drop is > 50 %, but it recovers to a value close to the initial voltage. This item fits with situation that cell voltage has significant change when the indenter applies load on cell, but voltage recovers close to initial voltage after test stops.
- If $V_{2\text{sec}}/V_{\text{init}} < 40 \%$ and $V_{\text{final}}/V_{\text{init}} > 70\%$ then $V_{\text{score}} = 3$.
- If $V_{2\text{sec}}/V_{\text{init}} \ge 40 \%$ and $V_{\text{final}}/V_{\text{init}} > 70\%$ then $V_{\text{score}} = 4$.
- If $V_{\text{5sec}}/V_{\text{init}} \ge 95 \%$ and no voltage recovery throughout the test then $V_{\text{score}} = 5$.
- 4. Weighted Coefficients wA, wB and wC are paired with T_{max} , T_{max} and V_{score} , respectively. The CHS is the linear combination of scores from these three components, the maximum temperature T_{max} , the maximum temperature T_{max} , and the voltage score V_{score} . To further normalize the final CHS values, in current study these three coefficients are assigned with constants that $wA=2.0^*cScale$, $wB=3.0^*cScale$ and $wC=2.0^*cScale$, cScale is a scale constant equal to 95/6 that works with constant cOffset (cOffset=5-cScale) to map final thermal runaway severity level into range 5.0–100.0.
- 5. Charge-related Coefficients wCap and wSOC are combined with V_{score} to include battery capacity counted by (mAH)/10000, and a percentage value of state of charge (SOC) into the risk severity/score calculation.

With all these terms defined, the final thermal runaway severity levels can be calculated with Eqs. 1–3. The maximum temperature T_{max} is the major criteria to divide the levels into three groups in Eq. (1). An upper threshold of 100.0 applies to all the severity level calculation. In addition to the calculated severity level ranging from 0 to 100, the battery thermal runaway severity level is further categorized into five groups, the very low (VL, Severity Level < 10), low (L, $10 \le \text{Severity Level} < 25$), moderate (M, $25 \le \text{Severity Level} < 75$), high (H, $75 \le \text{Severity Level} < 90$) and very high (VH, $90 \le \text{Severity Level} < 100$). As mentioned before, cell voltage

4	A	В	С	D	Е	F
1	FileName	Observed Score	Observed Score	Calculated Score	Capacity	SOC
51	OE-10Ahr-NMC-70SOC-cell6	Physical effect, rupture of pouch, smoke, gas	7	100.00	10000	70
		Moderate effect, extended joule heating, local				
52	OE-10AHr-NMC-40SOC-Cell4	reactions (no spread) – 3	3	50.83	10000	40
		Moderate effect, extended joule heating, local				
53	OE-10Ahr-NMC-40SOC-cell1	reactions (limited spread) - 4	4	54.99	10000	40
		Moderate effect, extended joule heating, local				
54	OE-10Ahr-NMC-0SOC-cell1	reactions (limited spread) - 4	4	37.09	10000	0

Fig. 7. the examples of calculated score in main.xlsx, Summary worksheet.

and temperature become less accurate and unreliable measures of thermal runaway severity, after the severity reaches 100.

Severity Level = 5,
$$If T_{max} < 40 \,^{\circ}C$$

= min $(S_{calc}, 100)$
= 100, $If T_{max} > 160 \,^{\circ}C$ (1)

$$S_{calc} = wA * \left(\frac{T_{max}}{160}\right)^{0.25} + wB * \left(\frac{\dot{T}_{max}}{200}\right) + wC * wCap * wSOC * V_{score} + cOffset$$
 (2)

$$= 1, \text{ if } V_{range}/V_{init} < 20\%$$

$$= 2, \text{ if } V_{range}/V_{init} > 50\% \text{ and } V_{final}/V_{init} < 20\%$$

$$V_{score} = 3, \text{ if } V_{2sec}/V_{init} < 40\% \text{ and } V_{final}/V_{init} < 20\%$$

$$= 4, \text{ if } V_{2sec}/V_{init} \ge 20\% \text{ and } V_{final}/V_{init} < 70\%$$

$$= 5, \text{ if } V_{5sec}/V_{init} > 95\%$$
(3)

All the calculated scores, along with cell properties such as capacity, SOC, observed thermal runaway effects, test file name are stored in Summary worksheet in main.xlsx. Figs. 2 and 7 show some of the calculated scores for different cells. Specially, examples in Fig. 7 indicate a strong correlation between the calculated thermal runaway score and the SOC of the 10 AHr NMC cells.

It might be helpful if you added an example of the implementation of the TR score calculation. There has been an extensive description of how that score is calculated but limited context for what it means.

Limitations

Some metadata of the battery properties, such as cell dimension, weight etc. are not included in this dataset.

Ethics Statement

The authors confirm that we have read and follow the ethical requirements for publication in Data in Brief and confirming that the current work does not involve human subjects, animal experiments, or any data collected from social media platforms.

CRediT Author Statement

Lianshan Lin: Conceptualization, Methodology, Investigation, Data curation, Formal analysis, Writing – original draft. **Jianlin Li:** Resources, Writing – review & editing. **Isabella Fishman:** Validation, Investigation, Data curation, Writing – review & editing. **Loraine Torre-Castro:** Conceptualization, Methodology, Resources, Data Curation, Writing – review & editing. **Yuliya Preger:**

Methodology, Resources, Data Curation, Writing – review & editing. **Valerio De Angelis:** Methodology, Resources, Data Curation, Software. **Irving Derin:** Software. **Xiaoqing Zhu:** Investigation, Data Curation. **Hsin Wang:** Conceptualization, Methodology, Resources, Investigation, Data curation, Formal analysis, Project administration, Supervision, Funding acquisition, Writing – review & editing.

Data Availability

Mechanically Induced Thermal Runaway for Li-ion Batteries (Original data) (Mendeley Data).

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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