

# Preventing Thermal Runaway Propagation in Lithium-Ion Batteries: A Holistic Review of Materials, Systems, and Predictive Strategies

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**Abstract.** Thermal runaway (TR) propagation in lithium-ion batteries (LIBs) poses significant safety risks in applications such as electric vehicles (EVs) and grid-scale energy storage systems. This comprehensive review synthesizes current research on TR mechanisms encompassing mechanical, electrical, and thermal abuse scenarios and evaluates mitigation strategies, including thermal barrier materials and advanced cooling systems. Experimental and computational studies underscore the efficacy of materials like aerogels, ceramic fibers, and phase-change composites, as well as active cooling methods such as liquid cooling and heat pipes, in suppressing TR propagation. Challenges in scalability, cost, and standardization are critically analyzed, with recommendations for interdisciplinary collaboration to bridge gaps between laboratory innovations and commercial deployment. Emerging solutions, including bio-derived aerogels, hydrogel composites, and hybrid cooling systems, are highlighted as sustainable pathways for next-generation battery safety.

**Keywords:** Thermal Runaway Propagation, Lithium-Ion Battery Safety, Battery Thermal Management, Thermal Barrier Materials, Phase Change Materials (PCMs), Machine Learning Prediction, Electric Vehicle Batteries, Battery Fire Mitigation.

## 1. Overview of Lithium-Ion Batteries

Lithium-ion batteries (LIBs) dominate modern energy storage due to their unparalleled energy density (150-250 Wh/kg), extended cycle life (1,000-2,000 cycles), and minimal self-discharge (~80% capacity retention after 30 days) [1–4]. Their operation relies on reversible lithium-ion intercalation between graphite anodes and transition-metal oxide cathodes (e.g., LCO, NMC, LFP), separated by porous polymer membranes in organic electrolytes [5–7]. Despite these advantages, thermal runaway (TR), triggered by mechanical/electrical abuse or thermal overstress, remains a critical safety challenge, evidenced by high-profile failures in aviation and electric vehicles [8–11].

## 2. Mechanisms of Thermal Runaway

Thermal runaway (TR) is a catastrophic failure mode characterized by uncontrolled heat generation, gas venting, and potential combustion. TR initiates at the cell level due to abuse conditions and propagates to adjacent cells through conductive, convective, or radiative heat transfer. Ref [12] investigated overcharge-induced thermal runaway (BTR) in lithium-ion batteries using real-world electric vehicle (EV) accident data. Key contributions by [12] included:

- **Real-scenario case analysis:** Examined a real EV battery thermal runaway accident caused by overcharging, leveraging data from China's National Monitoring and Management Platform.
- **Multi-stage characterization:** Divided overcharge into three stages (charged, fully charged, overcharged) and identified rising voltage inconsistencies and temperature spikes as precursors to BTR.
- **Electrochemical-thermal modeling:** Developed a multi-factor model incorporating environmental and driver behavior influences, validated via real-world data.
- **Probability model:** Proposed a rudimentary probabilistic framework to predict BTR risk, integrating factors like state-of-health degradation, weather, and driving patterns. This work [12] bridges laboratory-based research with real-world conditions, offering insights for improving EV battery safety protocols. Understanding the Thermal Runaway (TR) mechanisms is critical for designing mitigation strategies.

## 2.1. Mechanical Abuse

Mechanical abuse involves physical deformation or penetration of battery components, often resulting from collisions, crushing, or manufacturing defects.

**2.1.1. Collision and Crush:** Vehicle accidents can deform battery packs, leading to separator rupture, internal short circuits (ISC), or electrolyte leakage. Quasi-static compression tests reveal non-uniform cell deformation patterns, while dynamic impacts exacerbate localized damage due to high strain rates [13]. For example, studies on cylindrical LIBs demonstrate that plastic deformation of steel casings accelerates ISC risks during side impacts [5]. Collisions involving electric vehicles (EVs) can deform battery packs, leading to internal short circuits and thermal runaway. For instance, crash tests simulating EV impacts at 20 m height demonstrated significant smoke release and fire ignition due to mechanical abuse [14]. Real-world incidents, such as the Ft. Lauderdale EV crash, further underscore the risks of post-collision thermal runaway and reignition events [14].

**2.1.2. Penetration:** Nail penetration tests (e.g., GB/T 31485-2015) simulate ISC scenarios by puncturing cells with conductive probes. However, inconsistencies in test repeatability and the high energy density of modern LIBs complicate compliance with safety standards [13].

**2.1.3. Vibration-Induced Stress:** Vibration during vehicle operation can induce cumulative mechanical fatigue in LIBs, exacerbating structural degradation and increasing TR risks. Kjell and Lang [15] compared standardized vibration tests (e.g., IEC 62660-2, SAE J2380) with real-world EV measurements using Fatigue Damage Spectrum (FDS) and Shock Response Spectrum (SRS). Their findings revealed significant disparities in test protocols: (1) Most standards neglect low-frequency (<10 Hz) vibrations prevalent in field measurements, which dominate fatigue damage in large battery packs; (2) Vertical-direction testing alone (e.g., ECE R100) underestimates multi-axial stresses observed in harsh driving conditions; (3) Sinusoidal tests, while severe, may overemphasize high-cycle fatigue compared to broad-band random vibrations. These gaps highlight the need for vibration standards that better replicate real-world spectra to prevent latent mechanical failures that could trigger TR. Table 1 shows the vibration induced degradation in Lithium-Ion Batteries.

**Table 1: Vibration-Induced Degradation in LIB Cells**

| Cell Chemistry   | Vibration Profile          | DC Resistance Increase | Capacity Fade   | Critical Findings                                    |
|------------------|----------------------------|------------------------|-----------------|--|
| NCA 18650 [16]   | 10-year EU road simulation | Z-axis: 7.07%          | Not significant | Mechanical robustness across orientations            |
| NMC 18650 [17]   | 100,000 miles (SAE J2380)  | $\leq 128\%$           | $\leq 12.2\%$   | Severe degradation at 75% SOC + vertical orientation |
| General LIB [18] | 10–30 Hz EV simulation     | N/A                    | N/A             | 5°C surface temp. reduction during operation         |

**2.1.4. Real-World Vibration Exposure:** Electric vehicle battery packs endure complex multi-axis vibration spectra inadequately replicated by current standards (SAE J2380, ECE R100). Hooper and Marco [19] quantified in-vehicle vibrations across commercial EVs, revealing critical gaps: Dominant low-frequency content (<7 Hz) from suspension dynamics, Lateral (X/Y-axis) stresses exceeding vertical (Z-axis) loads, Urban/rural profiles inducing 10% higher energy (1-25 Hz) than motorways, High-frequency modes (>300 Hz) from powertrains unaddressed by  $\leq 200$  Hz standards.

- **Mechanical Degradation:** NCA cells subjected to 10-year equivalent vibration showed 7.07% DC resistance increase (indicating internal damage) despite other stable parameters [16]. NMC cells exhibited  $\leq 128\%$  DCIR rise, with severity escalating at 75% SOC and vertical (Z-Z) orientation [17].
- **Thermal Interactions:** Vibration enhances convective cooling (5°C reduction in surface temperatures at 20-30 Hz), yet 3C discharge still elevates temperatures to 50°C within 300 s [18]. This dual effect necessitates integrated thermal-mechanical design.

## 2.2. Electrical Abuse

**2.2.1. External Short Circuit (ESC):** ESC occurs when electrodes contact conductive materials (e.g., water immersion or damaged wiring), generating joule heating. Protective devices like fuses and positive temperature coefficient (PTC) components interrupt current flow to prevent overheating. External short circuit (ESC) faults can be described as a major safety hazard for lithium-ion battery applications. They can lead to overheating, cell damage, and even fire [20,21].

**2.2.2. Overcharging:** Overcharging drives excess lithium deposition at the anode, promoting lithium plating and dendritic growth, while cathode delithiation destabilizes oxide structures. This releases oxygen and accelerates electrolyte decomposition, particularly above 60°C, generating flammable gases (CO, H<sub>2</sub>)

and increasing internal pressure [22–24]. Ref [12] bridges laboratory and real-world conditions by analyzing an actual electric vehicle (EV) battery thermal runaway (BTR) incident caused by overcharging, using data from China's National Monitoring Platform. Key contributions include:

- **Staged Characterization:** Identifying voltage inconsistencies and temperature spikes as BTR precursors across three overcharge phases (charging, fully charged instant, overcharging).
- **Predictive Modeling:** Developing an electrochemical-thermal model validated against field data, integrated with a probabilistic framework to assess BTR risk from factors like state-of-health, weather, and driving behavior. This work advances safety protocols by quantifying real-world overcharge risks beyond controlled laboratory studies.

**2.2.3. Over-Discharging:** Voltage imbalances in series-connected packs can reverse cell polarity during over-discharge, generating abnormal heat. While less studied, this phenomenon poses risks in poorly balanced systems, particularly in low-voltage cells subjected to forced discharge by neighboring cells.

### 2.3. Thermal Abuse

Thermal runaway (TR) initiates through external heating or internal faults (e.g., internal short circuits, ISC), typically commencing with separator melting ( $\sim 130^\circ\text{C}$  for polyethylene) and cascading exothermic reactions. Recent studies reveal critical nuances in TR initiation and propagation:

- **Initiation Methods:** Kriston et al. [25] demonstrated inductive heating, a non-invasive technique leveraging alternating electromagnetic fields as an efficient TR trigger. By inducing eddy currents in conductive components, localized heating ( $\leq 4$  s) melts separators with minimal energy input ( $\sim 1\%$  of stored electrical energy), reproducibly initiating TR across cylindrical, pouch, and prismatic cells. Voltage fluctuations, gas venting, and rapid temperature escalation ( $400\text{--}800^\circ\text{C}$ ) ensued 10–40 s post-heating.
- **Cell Design Influence:** TR severity correlates more strongly with mechanical design (casing rigidity, venting mechanisms) than initiation energy. Prismatic cells exhibited explosive pressure release, whereas pouch cells showed delayed voltage collapse [25], aligning with prior findings on separator integrity [11,26].

#### 2.3.1. Reaction Mechanisms & Material Behavior

**2.3.1.1. SEI Decomposition:** The decomposition of the solid electrolyte interphase (SEI) occurs, releasing heat and flammable hydrocarbon gases [26].

**2.3.1.2. Electrolyte Vaporization:** At elevated temperatures, electrolyte components vaporize, generating gases such as  $\text{CO}_2$  and  $\text{C}_2\text{H}_4$ , which increases internal cell pressure [11].

**2.3.1.3. Cathode Decomposition:** Layered oxide cathodes undergo decomposition at high temperatures.  $\text{LiCoO}_2$  releases oxygen above  $180^\circ\text{C}$ , accelerating combustion. Ni-rich NMC811 cathodes release oxygen at around  $200^\circ\text{C}$  and account for approximately 81% of the total heat released. This occurs through two

primary reaction pathways: with ethylene carbonate (16%) and the lithiated anode (65%) [27]. Gas evolution and thermal reactivity are further exacerbated at higher states of charge (SOC) [28].

**2.3.1.4. Heating Dynamics & Propagation:** Gagnon et al. [29] revealed that faster heating rates (0.5°C/s) reduced TR initiation time by 50% in 63 Ah NMC pouch cells versus slower rates (0.2°C/s), though peak temperatures remained consistent (~756°C). Propagation delays increased with heating rates due to steeper thermal gradients, highlighting limitations of lumped thermal models. Kim et al. [30] identified stochastic TR stages in NCM811 pouch cells: initial gas/flame ejection (venting speeds: 123.8 m/s), flame extinction, multi-point ignition, and stable jet formation (20-40 m/s). Ejected high-temperature particles (e.g., metal oxides) acted as ignition sources. Aiello et al. [31] observed eight distinct TR phases in constrained NMC-LMO modules, with radial ISC propagation driven by electrolyte expansion. Mechanical constraints altered adjacent-cell failure delays (10-18 s), while voltage drops preceded temperature spikes by ~3 s.

**2.3.1.5. Cell Format & Capacity Effects:** Peng et al. [32] showed that heating methods significantly influence TR: electric plates induce earlier TR with suppressed combustion, while ovens trigger violent jet flames. Larger cells (180 Ah) delayed TR onset (2163 s vs. 967 s for 60 Ah) but produced higher explosive gas emissions (H<sub>2</sub>,CO). Wang et al. [33] observed TR initiation at pouch cell edges under surface heating, consistent with low thermal tolerance of edge materials (e.g., polypropylene adhesives, ~170°C [31]). Maloney [34] reported faster TR propagation in pouch versus cylindrical cells due to enhanced thermal coupling. Propagation kinetics exhibited strong SOC dependence, with pouch cells showing 53-83°C higher onset temperatures at 20% SOC than at 100% SOC due to reduced electrochemical reactivity [34].

**2.3.1.6. Detection & Modeling Advances:** Embedded PTC sensor arrays detect SEI decomposition at 67°C, enabling early intervention and post-cooling reuse [35]. Recurrent Neural Networks (RNNs) achieve high-fidelity surface temperature estimation under dynamic loads, facilitating preemptive cooling [36]. Multiphysics models (e.g., Domalanta and Paraggua [37]) identify cathode-electrolyte reactions as dominant heat sources ( $5.7 \times 10^8$  kW/m<sup>3</sup> at 423.15 K) and validate material-level strategies. Wang et al. [33] further demonstrated 3D models predicting heat accumulation at sealing edges.

## 2.4. Thermal Runaway in All-Solid-State Batteries (ASSBs)

Recent studies challenge assumptions of inherent safety in solid-state batteries by revealing distinct thermal runaway (TR) pathways:

- **Sulfide Electrolytes:** Glassy-ceramics (e.g., Li<sub>3</sub>PS<sub>4</sub>) react with cathode-released O<sub>2</sub> at ~200°C, generating toxic SO<sub>2</sub> and extreme heat (~2100 J·g<sup>-1</sup>) via gas-solid reactions [38].
- **Electrolyte Comparison:** Oxide/garnet electrolytes (e.g., LLZTO) exhibit higher TR onset temperatures (e.g., 251.1°C vs. liquid LIBs: 80-120°C) and reduce total TR energy by 70-80% by suppressing combustion. Sulfide/polymer systems retain significant TR risks under oxygen-rich conditions [39].

- **Critical Risks:** Violent combustion occurs even in inert atmospheres [38], while reactive cathode-electrolyte interfaces (e.g., sulfide-NCM811) accelerate exothermic reactions at 200°C [39]. Toxic SO<sub>2</sub> release during GSR poses environmental hazards [38].
- **Design Imperatives:** TR mitigation requires cathode/electrolyte co-design to suppress cross-talk reactions [38] and optimized interfaces (e.g., oxide additives) to delay propagation [39]. These findings underscore that solid-state batteries are not intrinsically safer than conventional Li-ion systems and demand tailored material engineering for thermal stability [38,39].

## 2.5. Impact of Aging on Thermal Runaway Mechanisms

Recent work by Preger et al. [40] synthesizes critical insights into how aging alters lithium-ion battery (LIB) safety under thermal, electrical, and mechanical abuse. Preger et al. [40] synthesize how aging alters lithium-ion battery safety under abuse conditions:

- **Degradation Mechanisms:** Microcracking, transition metal dissolution (Mn, Ni), and SEI/CEI growth reduce thermal stability. High-temperature aging accelerates cathode phase transitions and cracking, while low temperatures promote Li plating and SEI recomposition, increasing heat generation and thermal runaway (TR) susceptibility [41].
- **Thermal Abuse:** Lithium plating (from low-T cycling) lowers TR onset by  $\leq 70^\circ\text{C}$  but reduces peak temperatures due to capacity fade. High-T aging delays self-heating via SEI stabilization.
- **Electrical Abuse:** Aged 18650 cells with safety devices (e.g., CID) activate earlier during overcharge, preventing TR. Aged pouch cells without devices show delayed TR with lower peak temperatures ( $\sim 360^\circ\text{C}$  vs.  $>900^\circ\text{C}$ ). External shorts exhibit minimal aging impact.
- **Mechanical Abuse:** Aged pouch cells require greater intrusion for short circuits; cylindrical cells show delayed TR post-penetration due to electrolyte dry-out.
- **Module-Level:** Reduced TR propagation risk in aged modules from earlier CID activation and lower energy content, though design-dependent. This work underscores the need for aging-aware safety protocols, especially in second-life applications where degradation alters failure dynamics [40].

## 3. Lithium-Ion Battery Pack Architecture

LIB packs integrate hundreds to thousands of cells into modules housed within thermally resistant enclosures [42]. Aluminum or polymer casings provide structural support, electrical insulation, and chemical resistance. System-level safety strategies focus on delaying TR propagation, as suppressing initiated TR is nearly impossible. Innovations like aluminum-doped NMC cathodes improve intrinsic stability, but thermal barriers and active cooling systems remain critical for containment [10,11,43]. Prismatic pouch cells are often preferred in modern EVs due to their large surface area for heat dissipation, although cylindrical cells still dominate due to ease of mass production [44]. Recent advances in hybrid thermal management systems (TMS), combining phase-change materials (PCMs) with liquid cooling or heat pipes, have demonstrated enhanced heat dissipation and uniformity, reducing TR risks under high discharge rates [43].

## 4. Mitigation Strategies Against Thermal Runaway

**4.1. Active Suppression & Monitoring:** Integrated fire suppression systems (e.g., water mist/spray, 12-13 L capacity) delay cell-to-cell propagation by reducing peak temperatures by 30% through hotspot cooling [14]. When combined with thermal barriers (aerogels, ceramic fibers) [45,14] and embedded PTCR sensors enabling real-time monitoring and current interruption [35], they form multi-layered defenses.

**4.2. Material Innovations:** Cathode-electrolyte compatibility optimization is critical, as cathode decomposition dominates TR heat generation [37]. Advanced coatings (e.g., Al-doped NMC) can suppress exothermic reactions.

**4.3. Module Design Optimization:** Key parameters significantly impact propagation:

- **Cell spacing:**  $\geq 2$  mm gaps reduce adjacent cell temperatures by  $\sim 30\%$  [46]
- **Tab configuration:** Branched (M-type) tabs minimize electrical draining into failed cells versus serpentine designs [46]
- **Insulation:** Radiant barriers limit adjacent temperatures to critical thresholds ( $< 150^\circ\text{C}$ ) that suppress propagation [46]
- **Vent orientation:** Side-facing vents in prismatic cells require reinforced thermal barriers due to directional ejecta [46].

**4.4. Aerogel-Based Thermal Barriers:** Silica aerogels, with ultra-low thermal conductivity ( $\kappa = 0.015\text{-}0.025 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ ), represent the benchmark for suppressing heat transfer in lithium-ion battery packs. Recent innovations focus on enhancing their multifunctional capabilities:

- **Hybrid Architectures:** Yu et al. [47] engineered a copper/aerogel/copper sandwich composite (STI board;  $\kappa = 0.031 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ ) that delays thermal runaway (TR) propagation  $> 6$  hours in NMC modules. This design synergistically: Suppresses convection (63.5% airflow reduction), Blocks radiation (emissivity: 0.1; 35.1% lower heat absorption), Maintains structural stability under thermal stress (sustaining a  $540^\circ\text{C}$  gradient at  $750^\circ\text{C}$ ).
- **Alternative Formats & Performance:** Aerogel blankets ( $\kappa = 0.021\text{-}0.077 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$  across  $20\text{-}600^\circ\text{C}$ ) exhibit hydrophobicity (contact angle:  $138^\circ$ ), compressive strength (1,700 kPa), and vibration resistance, enabling scalable deployment [48].
- **Microstructural Optimization:** Hoseini et al. [49] demonstrated that reduced porosity (91% in Cryogel® Z) while fiber choice negligibly impacts insulation efficacy. Their validated multiscale model confirms pore-dominated heat transfer, guiding future material design. Critical Perspective: While aerogels enable multi-modal heat inhibition (conduction, convection, radiation), industrial adoption hinges on resolving cost-performance tradeoffs. Hybrid metallic-aerogel systems show exceptional promise but require manufacturing scalability for widespread integration [47,50,51].

**4.5. Ceramic Fibers:** Alumina-silicate fibers (0.05-0.1 W/m·K) provide fire resistance and thermal shock resilience. Ceramic wool layers delay heat propagation by 5-10 minutes in 18650 cell modules [52]. Nambisan et al. [45] demonstrated that a 50-mm ceramic wool layer limited cold-side temperatures to below 150°C under 1360°C flame exposure. Hybrid configurations combining ceramic wool with graphite or aerogels showed improvement in insulation efficiency compared to standalone materials [45]. Recent advances in electrospun ceramic nanofibers demonstrate exceptional thermal insulation and flexibility. Zhao et al. [53] developed flexible Al<sub>2</sub>SiO<sub>5</sub> nanofiber membranes via electrospinning, achieving ultra-low thermal conductivities of 0.03487 W/(m·K) at -25°C and 0.07384 W/(m·K) at 800°C. These membranes delayed thermal runaway (TR) propagation by 1608 s in 21700 battery modules and improved low-temperature performance, maintaining 2.22 Ah capacity at -25°C (vs. 1.67 Ah for unwrapped cells). Their high-temperature stability (resisting 1300°C flames) and mechanical flexibility (0.86 MPa tensile strength) make them promising for hybrid thermal management systems. Recent advances in separator design, such as SiO<sub>2</sub>-grafted polyethylene membranes and polyimide nonwoven fabrics, demonstrate improved thermal stability (withstanding >250°C) and reduced shrinkage during thermal events [54]. These innovations complement ceramic fiber barriers by addressing both intrinsic cell safety and module-level heat propagation.

#### 4.6. Active Cooling Strategies for Thermal Runaway Mitigation

Active cooling systems constitute critical interventions for dissipating heat prior to thermal runaway (TR) initiation. Recent advances demonstrate significant efficacy but reveal inherent design compromises.

##### 4.6.1. Immersion Cooling & Thermal Optimization:

- **Dielectric Fluids:** Han et al. [55] empirically demonstrated dielectric fluid immersion (E5-TM410) sustains temperatures <45°C at 4C discharge (heat transfer coefficient: >2200 W·m<sup>-2</sup>·K<sup>-1</sup>). However, suboptimal flow paths exacerbate temperature gradients, undermining electrical performance.
- **Fin Geometry:** Triangular fins enhance thermal uniformity and Nusselt numbers, reducing peak temperatures by 4.45% versus finless designs. Optimized aspect ratios (A/B=4.304) further limit temperatures to 35.07°C at 5C [56].

##### 4.6.2. Flow Dynamics & Adaptive Control:

- **Non-Monotonic Efficacy:** Jindal et al. [57] computationally revealed increased coolant flow initially accelerates TR propagation via convective redistribution, necessitating critical thresholds for suppression.
- **Intermittent Spraying:** Zhang et al. [58] identified optimal spray intervals (20s pulse/0.5 duty cycle) to limit adjacent cells to <150°C by minimizing film thickness and maximizing evaporation. A two-stage hybrid strategy: rapid flame suppression followed by sustained cooling, proved most effective.

- **Hybrid System Integration:** Liquid cooling, heat pipes, and phase-change materials (PCMs) synergize with thermal barriers to achieve  $<5^{\circ}\text{C}$  pack uniformity [43]. Parametric optimization of flow control and geometry remains essential to balance heat extraction efficiency against parasitic losses.

#### 4.7. Fire-Extinguishing Agents for LIB Fires

Fire-extinguishing agents constitute critical last-line defenses against thermal runaway (TR)-induced combustion in lithium-ion batteries (LIBs), complementing preventive thermal barriers and cooling systems. LIB fires present unique challenges: high temperatures ( $>800^{\circ}\text{C}$ ), multi-class fire behavior (A-D), and persistent re-ignition risks. Effective agents require high heat capacity (e.g., water-based systems [59]), electrical insulation (e.g., gaseous agents [59]), and wettability for module penetration. Water-based agents are recommended for large-scale LIB fires due to unmatched cooling efficacy, despite conductivity concerns in integrated packs. Their synergy with thermal barriers (e.g., aerogels [51]) and active suppression (e.g., mist systems [14]) enables multi-stage TR containment. Future development must address: 1. Insulating agent formulations to mitigate short-circuit risks, 2. BMS-integrated deployment for real-time response to venting or thermal anomalies [59].

### 5. Machine Learning-Driven Prediction and Mitigation of Thermal Runaway

**5.1. Paradigm Shift to Data-Driven Safety:** Recent advancements have established machine learning (ML) as a transformative tool for predicting and mitigating thermal runaway (TR) in lithium-ion batteries. By leveraging minimal experimental data, ML models bypass resource-intensive physical testing while achieving high-fidelity simulations of complex thermal-electrochemical interactions. Masalkovaitè et al. [60] demonstrated that support vector machines (SVMs) trained on ejected mass and cell metadata predict heat release variability during TR for commercial 18650/21700 cells with similar chemistries. This approach reduces calorimetry needs by  $>80\%$  (requiring only 0–5 FTRC tests) and accelerates safety screening, though validation for radically new chemistries (e.g., LFP, silicon anodes) remains untested.

**5.2. Digital Twin Frameworks for Proactive Management:** Digital twins (DTs) represent the pinnacle of this evolution, integrating physics-based models, real-time sensor data, and ML to create dynamic virtual replicas of battery systems.

**5.2.1. Architectural Innovations:** Wang et al. [61] developed a dual-agent deep learning framework combining Artificial Neural Networks (ANNs) and Convolutional Neural Networks (CNNs) to predict thermal runaway propagation times and 2D temperature fields in battery packs. Trained on 36 CFD simulations, it achieves high accuracy ( $R^2>0.99$  for temperatures,  $<10\%$  error in propagation time for in-database scenarios) with real-time inference ( $<1$  s/scenario), representing a  $>99.9\%$  computational speedup over conventional CFD. However, accuracy degrades for extrapolated conditions (e.g.,  $\sim 30\%$  error in propagation time at  $55^{\circ}\text{C}$  ambient). Shen et al. [62] developed a CNN-based DT for large packs, using Bayesian-optimized neural networks to predict spatiotemporal thermal fields in 2.92 s (MAE:  $<0.73^{\circ}\text{C}$ ). Its ultra-low computational footprint (3.31 MFLOPs) enables edge deployment on automotive hardware.

**5.2.2. Industrial Implementation Frameworks:** Dubarry et al. [63] established a holistic framework for scalable battery digital twins, emphasizing hybrid physics-ML modeling, blockchain-enabled lifecycle traceability, and Bayesian uncertainty propagation for adaptive parameterization. Applications include root-cause analysis of manufacturing defects and probabilistic safety forecasting. Complementarily, Singh et al. [64] developed a PyBaMM-based implementation workflow using DFN electrochemical models, with semi-empirical parameter updates via cycling data for SOC/SOH estimation and degradation tracking.

### 5.3. Advanced Neural Network Architectures

**5.3.1. Predictive Modeling:** Lekoate et al. [65] demonstrated that Layer Recurrent NNs (LR-NNs) outperform Elman and Feedforward NNs in forecasting thermal runaway (TR) temperatures (MSE: 0.840; RMSE: 0.917). State of Charge (SOC) was identified as a dominant input, where higher SOC increases Gibbs energy ( $\Delta G$ ), accelerating cathode decomposition and combustion reactions that elevate TR risk. Zhou et al. [66] applied ANNs to predict cathode decomposition under reductive gases, using thermochemical data (TGA/DSC) to achieve  $R^2 = 0.73$  for degradation onset temperatures. An analytic hierarchy process (AHP) weighted risk parameters, enabling quantitative cathode safety scoring.

**5.3.2. Physics-Informed Hybrids:** Shen et al. [67] embedded thermal-physical equations into an LSTM network, creating a Physics-Informed NN (PINN) with exceptional temperature estimation accuracy (RMSE:  $<0.6^\circ\text{C}$ ; MAE:  $<0.5^\circ\text{C}$ ). Entropy effects were modeled via regional equivalent resistance, enhancing interpretability with minimal training data. Lyu et al. [68] fused multi-particle electrochemical-thermal-mechanical models with real-time data assimilation, achieving MAEs of  $\leq 15$  mV for voltage (constant-current) and  $\leq 0.35^\circ\text{C}$  for temperature, enabling high-fidelity state monitoring in packs.

## 6. Conclusion

Thermal runaway (TR) propagation remains a paramount safety challenge for lithium-ion battery (LIB) systems, particularly as energy densities escalate to meet the demands of electric vehicles and grid-scale storage. This review has synthesized the complex phenomenon of abuse mechanisms: mechanical deformation, electrical faults, and thermal overstress, and evaluated the evolving landscape of mitigation strategies across material, system, and predictive domains.

### 6.1. Key Findings Synthesis

- **Material Innovations Show Promise but face barriers:** Advanced thermal barrier materials like silica aerogels, electrospun ceramic nanofibers, and multifunctional phase-change composites (PCCs) demonstrably delay TR propagation by impeding multi-modal heat transfer (conduction, convection, radiation). Hybrid designs (e.g., metallic-aerogel sandwiches, flame-retardant hydrogel-PCM composites) offer synergistic performance exceeding individual components. However, significant hurdles in cost, manufacturing scalability, mechanical robustness under vibration, and long-term stability impede widespread commercial adoption. The inherent TR risks

revealed in all-solid-state batteries necessitate dedicated material co-design strategies, highlighting that safety is not intrinsic but engineered.

- **System-Level Design is Critical for Containment:** Preventing initiated TR is nearly impossible; thus, system architecture focuses on delaying propagation. Optimized pack design parameters including sufficient cell spacing, strategic vent orientation, branched tab configurations, and robust module insulation are as crucial as material selection. Active cooling systems are also essential for managing operational heat and pre-TR hotspots, but their efficacy is highly dependent on flow dynamics, geometry optimization, and integration with passive barriers. Hybrid thermal management systems (HTMS) combining active cooling with passive insulators (such as aerogels, ceramifiable silicones, mica) represent the most effective approach, demonstrably reducing peak temperatures and TR propagation risk.
- **Prediction and Proactive Mitigation are Emerging Frontiers:** Machine Learning and Digital Twin technologies are revolutionizing TR safety. Physics-informed neural networks, hybrid ANN-CNN models, and data-mechanism fusion frameworks enable high-fidelity prediction of TR initiation, propagation dynamics, and spatiotemporal thermal fields with unprecedented speed and accuracy.

## 6.2. Persistent Challenges and Critical Barriers

- **Cost-Scalability-Performance Trilemma:** The most effective materials (e.g., high-purity aerogels, multifunctional PCCs) often suffer from prohibitively high costs or complex manufacturing, hindering deployment in cost-sensitive mass markets like automotive.
- **Standardization and Validation Gaps:** Critical inconsistencies exist in international abuse testing protocols (mechanical force thresholds, electrical termination criteria, fire exposure realism). The lack of harmonized standards for validating novel materials and systems under realistic multi-abuse and aged conditions creates uncertainty for manufacturers and regulators. Standardization efforts lag behind rapidly evolving cell formats and chemistries.
- **Interfacial and Integration Challenges:** Optimizing interfaces between different mitigation layers (e.g., barrier material to cell casing, cooling plate to PCM) and ensuring compatibility with BMS sensors/actuators is critical for system-level efficacy but often overlooked in component-focused research.
- **Sustainability Imperative:** The environmental footprint of mitigation materials (e.g., mining for ceramics, synthetic polymers) requires greater attention. Bio-derived alternatives (cellulose aerogels, bio-chars) offer promise but need performance and cost parity improvements.

## 6.3. Future Research and Development Priorities

### 6.3.1. Next-Generation Sustainable Materials: Accelerate development and scale-up of:

- Cost-effective, high-performance insulators: Advanced bio-aerogels, scalable ceramic nanofiber production, multifunctional intumescent coatings.

- Inherently Safer Chemistries & Interfaces: Flame-retardant electrolyte additives, engineered artificial SEI/CEI layers, and co-designed all-solid-state batteries (ASSB) cathode/electrolyte pairs specifically targeting TR suppression.
- Anisotropic Thermal Management Materials: Combining high in-plane conductivity (for operational heat spreading) with ultra-low through-plane conductivity (for TR blocking).

### 6.3.2. Intelligent, Integrated Safety Systems

- Embedded Multi-Parameter Sensing: Development and integration of low-cost, robust sensors (gas, pressure, distributed temperature/PTC, strain) for early fault detection.
- ML-Driven Adaptive Control: Tight coupling of predictive Digital Twins with BMS to enable real-time modulation of cooling, load, and isolation strategies based on predicted TR risk and pack condition.
- Multi-Layer Hybrid Mitigation: Optimized integration of material barriers (aerogel/ceramic), active cooling (variable flow liquid/immersion), and suppression agents (targeted mist/spray) triggered by predictive models.

### 6.3.3. Harmonized Standards and Lifecycle Validation

- Unified International Protocols: Develop realistic, multi-stress abuse tests (e.g., combined vibration, thermal shock, overcharge) representative of field failures, incorporating aged cells and large-format/module-level validation. Protocols must evolve with new technologies (ASSBs).
- Probabilistic Risk Assessment Frameworks: Integrate real-world data (like EV telematics used in Ref [12]) with lab-derived models to quantify TR likelihood under diverse operating conditions and aging states.
- Lifecycle Sustainability Assessment: Include environmental impact analysis (LCA) as a core criterion in evaluating TR mitigation solutions from material sourcing to end-of-life.

Achieving inherently safer high-energy-density LIB systems necessitates a paradigm shift from isolated component improvements to holistic, system-level co-design. This requires unprecedented collaboration across disciplines: chemists and material scientists developing next-generation intrinsically stable materials and sustainable barriers; mechanical and thermal engineers designing optimized packs and hybrid thermal management systems; electrical engineers and computer scientists advancing embedded sensing and intelligent BMS; and policymakers/standardization bodies establishing rigorous, harmonized validation frameworks. The convergence of thermally resilient materials, intelligently controlled thermal architectures, predictive digital tools, and robust international standards is not merely desirable but essential to unlock the full potential of lithium-ion batteries for a sustainable electrified future, ensuring safety is engineered from the molecular level to the full pack system.

## Author Contributions

Author 1 conceptualized the study, designed the structure of the review, conducted the literature survey, analyzed and synthesized the findings, and wrote the manuscript.

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## Conflict of Interest

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## Data Availability Statements

The datasets generated and/or analyzed during the current study are available from the corresponding author on reasonable request.

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