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# Comprehensive Review of Emerging Lithium and Sodium-Ion Electrochemical Systems for Advanced Energy Storage Applications

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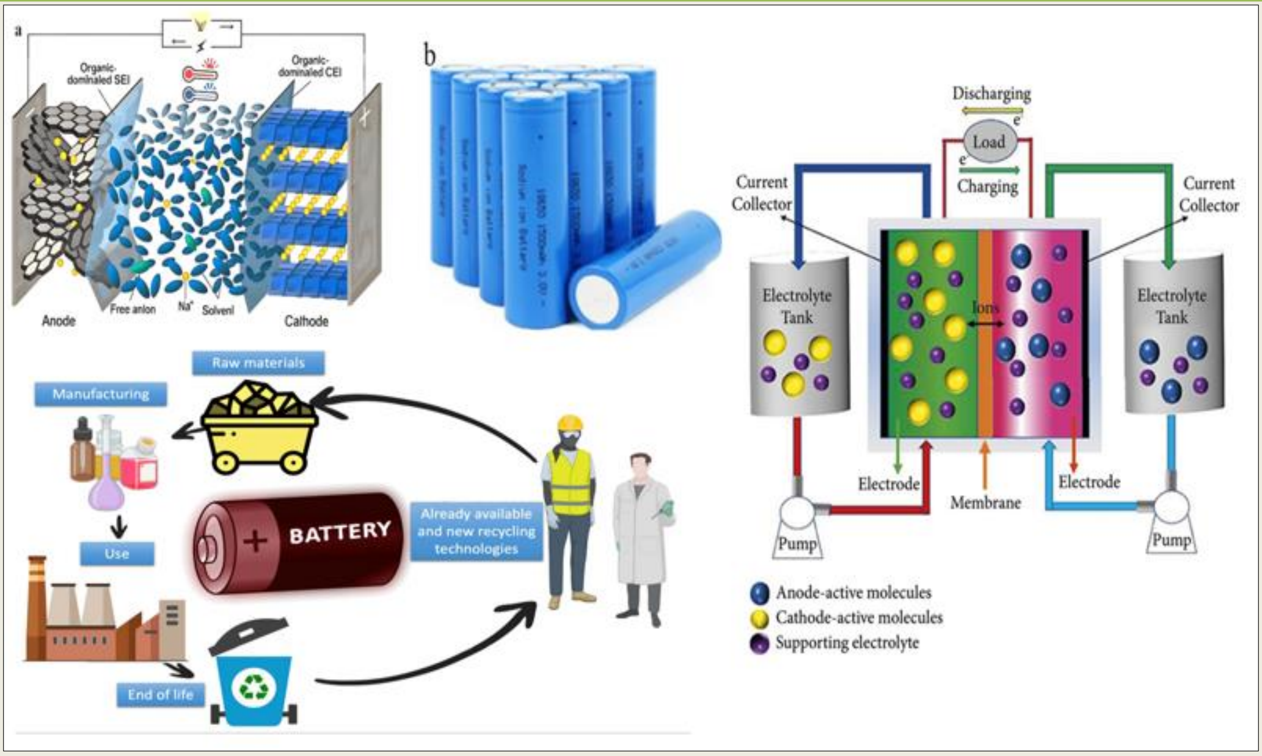
**Abstract** **Review Article**




**Graphical Abstract**

The need for effective, scalable, and sustainable energy storage solutions has increased due to the quick spread of electric cars, portable gadgets, and renewable energy sources. Because of their extended cycle life, high energy density, and established manufacturing infrastructure, lithium-ion (Li-ion) batteries have long dominated the energy storage market. However, the hunt for substitute technologies, especially sodium-ion (Na-ion) batteries, which take advantage of the cheap and plentiful sodium, has accelerated due to the limited supply and growing expense of lithium resources. This

paper thoroughly analyzes Li-ion and Na-ion electrochemical systems, emphasizing the fundamental ideas, current developments, and new difficulties related to these technologies. Important elements, including electrolytes, separators, cathode and anode materials, and electrode/electrolyte interactions, are thoroughly investigated. Innovative material advancements that improve battery performance and safety are highlighted, such as layered oxide cathodes, alloy and conversion-type anodes, solid-state and gel polymer electrolytes, and surface modification methods. The energy density, rate capability, cycle stability, environmental effect, and cost-efficiency of Li-ion and Na-ion systems are compared. The analysis also examines the commercialization and scaling prospects of next-generation batteries, emphasizing initiatives in recycling, green synthesis, and smart grid integration. The environmental and techno-economic effects of switching from lithium to sodium-based chemistry are specifically discussed. This review's main goals are to summarize existing knowledge, pinpoint technological gaps, and delineate future research goals that might propel the creation of sustainable, high-performance electrochemical energy storage systems suited for a variety of cutting-edge applications.
**Keywords:** Lithium-Ion Batteries (LIBs), Sodium-Ion Batteries (SIBs), Electrochemical Energy Storage, Cycle Life, Next-Generation Batteries, Sustainable Energy Storage, Battery Performance Optimization, Emerging Electrode Materials, Sodium-Ion Battery Chemistry.


# INTRODUCTION

As the world struggles with rising global energy demands and increasing pressure to decarbonize, the race for next-generation energy storage technologies is picking up speed (Mann *et al*., 2020). While switching from fossil fuels to renewable energy sources like solar and wind is necessary to fight climate change, the intermittent nature of these energy sources highlights the urgent need for effective, scalable, and sustainable storage solutions. While lithium-ion batteries are currently the industry standard, they have limitations in terms of raw material availability, energy density, safety, and environmental impact (Oliveira *et al*., 2015). As a result, researchers and industries around the world are making significant investments in alternatives like solid-state batteries, metal-air batteries, sodium-ion technologies, and even more innovative approaches like flow batteries and supercapacitors. Higher energy densities, quicker charging speeds, cheaper prices, and less dependence on vital minerals like cobalt and lithium are just a few of the distinct benefits that each of these new technologies has to offer (Placke *et al*., 2017). The search for safe, localized energy storage technologies that support national sustainability objectives has also been fuelled by the geopolitical tensions surrounding resource supply chains. In addition to improving knowledge, this global technology sprint aims to redefine energy justice, economic resilience, and climate responsibility (Sarkodie *et al*., 2023). Energy storage innovation is a key component of the clean energy revolution of the twenty-first century, since the conclusion of this race will influence future electric mobility, grid dependability, and the overall decarbonization landscape (Asif *et al*., 2024).

The distinctive electrochemical characteristics of lithium, including its high energy density, low weight, and superior cycle performance, have contributed to its domination in the battery industry, especially for use in consumer electronics, electric vehicles (EVs), and grid-scale energy storage (Gür *et al.,* 2018). Because of their maturity, efficiency, and continuous improvements in anode, cathode, and electrolyte technology, lithium-ion batteries (LIBs) have emerged as the industry standard. However, the limited geographic distribution of lithium reserves, mostly concentrated in areas like the Lithium Triangle in South America, Australia, and parts of China, has led to significant concerns about sustainability, geopolitical supply chain risks, and rising costs as a result of the world's reliance on lithium (Sanchez-Lopez *et al.,* 2023). Lithium mining and processing use a lot of energy and present environmental problems, such as water use and ecological damage. These difficulties, together with the EV market's growing demand, have spurred a global hunt for other battery chemistries. Because of sodium's availability, affordability, and chemical resemblance to lithium, sodium-ion batteries (SIBs) have become a very promising substitute among these (Zhao *et al.,* 2023). Because sodium is abundant in saltwater and the earth's crust, it is a more ecologically friendly and geopolitically secure choice. Although SIBs are currently less energy dense than LIBs, the performance gap is closing fast due to technical advancements in solid-state topologies, electrolyte formulation, and electrode materials (such as hard carbon anodes and layered oxide or Prussian blue analog cathodes). SIBs are perfect for large-scale stationary storage systems where size and weight are less important, since they also have clear advantages in terms of thermal stability, safer working conditions, and greater performance at low temperatures (Gao *et al*., 2024).

Globally, major battery manufacturers and research institutes, including CATL, Faradion, and Natron Energy, are making significant investments in creating pilot production lines, integrating SIBs into commercial products, and scaling up sodium-ion technology (Jayaraman *et al*., 2024). The emergence of sodium-ion batteries marks a dramatic change in the energy storage business as global markets look for robust and diverse supply chains and demand grows to switch to more sustainable technologies. The growing maturity of sodium-ion alternatives is establishing a significant complementary niche, even if lithium is unlikely to be completely overtaken anytime soon, particularly in applications where ultra-high energy density is crucial (Deshmukh *et al*., 2025). A more pluralistic battery ecosystem, where several chemistries coexist to satisfy the various demands of a decarbonizing world, is beginning with this progression. The design, functionality, and promise for scalable, sustainable energy storage of lithium-ion and sodium-ion electrochemical systems are the main topics of this thorough analysis. The article discusses both solid-state and liquid-based topologies and covers a wide range of components, such as electrodes, electrolytes, separators, and binders. Particular focus is placed on the new materials, structural engineering techniques, and developing chemistries that are influencing the development of high-performance energy storage devices in the future (Pomerantseva *et al*., 2019). The study presents a comprehensive picture of the changing energy storage environment by combining ideas from theoretical models, experimental data, and techno-economic evaluations. To evaluate and contrast the electrochemical performance, cost, material availability, and environmental effects of lithium-ion and sodium-ion battery systems.

**Electrochemical Fundamentals**

**Lithium vs Sodium – A Tale of Two Ions**

The elemental and ionic features of lithium ($Li^+$) and sodium ($Na^+$) ions, which both have a direct impact on how well they operate in contemporary energy storage systems, mold their electrochemical activity into an engaging story (Kundu *et al*., 2015). With an atomic number of three and an atomic mass of around 6.94 u, lithium is a light alkali metal and the third element in the periodic table. Although sodium is a member of the same group and is somewhat heavier (atomic number: 11; atomic mass: about 22.99 u), its bigger atomic and ionic sizes cause it to behave very differently in electrochemical systems. Since $Li^+$ ions have a radius of around 0.76 Å while $Na^+$ ions have a radius of about 1.02 Å, $Li^+$ ions are more compact and have a greater charge density. Stronger solvation results from improved electrostatic interactions with polar solvent molecules caused by this increased charge density (Gabdoulline *et al*., 1996). The energy of solvation, which can be estimated as ΔGsolv∝−rz2, is therefore noticeably worse for $Li^+$ than for $Na^+$. This affects the ion's capacity to take part in quick redox processes, though, because it also leads to increased desolvation energy penalties at the electrode interface. Lithium has a greater negative standard reduction potential from a redox perspective ($E_{Li+/Li∘}$ = −3.04V), compared to sodium (ENa+/Na∘ = −2.71V), increasing the electrochemical reactivity of lithium and its capacity to generate greater cell voltages. The Nernst equation may be used to represent the connection between electrode potential and concentration:

$$E = E^0 - RT/nF \text{ In } Q$$

Higher energy density for lithium-ion batteries is a direct result of $Li^+$'s larger negative redox potential. Lithium again has the advantage in terms of ion mobility because of its smaller mass and size. The Einstein relation states

$$\mu=Dq/kT$$

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$$\kappa=i\sum zi2ci\mu iF$$

Each ion species' charge, concentration, and mobility, in that order. Practical benefits of sodium include its higher natural abundance, less cost, and compatibility with aluminum current collectors rather than the more costly copper utilized in lithium systems. Sodium-ion batteries may have a lower voltage and energy density, but they are promise for large-scale applications like grid storage because of their affordability and scalability. In conclusion, despite their chemical similarities, lithium and sodium exhibit distinct electrochemical behaviors that are based on their atomic and ionic characteristics. This comparison also reveals important trade-offs for developing next-generation battery technology.

## MATERIAL MATTERS

**Spicy Trends in Anode and Cathode Innovations**

The materials underlying next-generation lithium and sodium-ion batteries are experiencing a revolution in the quickly changing field of electrochemical energy storage, with anode and cathode advances taking center stage (Zhang *et al*., 2024). The transition from conventional graphite to cutting-edge substitutes like hard carbon and MXenes represents a daring step forward in the anode's optimization of anode energy density, rate performance, and cycle stability. MXenes 2D transition metal carbides and nitrides—offer remarkable conductivity and surface functionalization potential, opening up new possibilities in fast-charging applications, while hard carbon, with its distinct porous structure and high sodium storage capacity, is particularly important for sodium-ion systems. At the same time, cathode materials are becoming more complicated and effective, incorporating polyanionic chemicals like phosphates and sulfates in addition to traditional layered oxides. Which improves voltage output and thermal stability (Ling *et al*., 2021). An additional layer of architectural complexity is added by the introduction of P2 and P3-type layered structures in sodium-ion batteries, which provide better structural reversibility and rate capability. The development of dual-ion and mixed-metal cathode frameworks, such as lithium-sodium hybrid cathodes, which combine the best aspects of both chemistries to create synergistic electrochemical performance, is the true spice in this growing materials matrix. In order to meet the needs of future grid, electric car, and wearable applications, these hybrid systems promise to overcome the drawbacks of single-ion storage and open the door for reliable, scalable, and high-energy-density storage options (Boaretto *et al*., 2021).

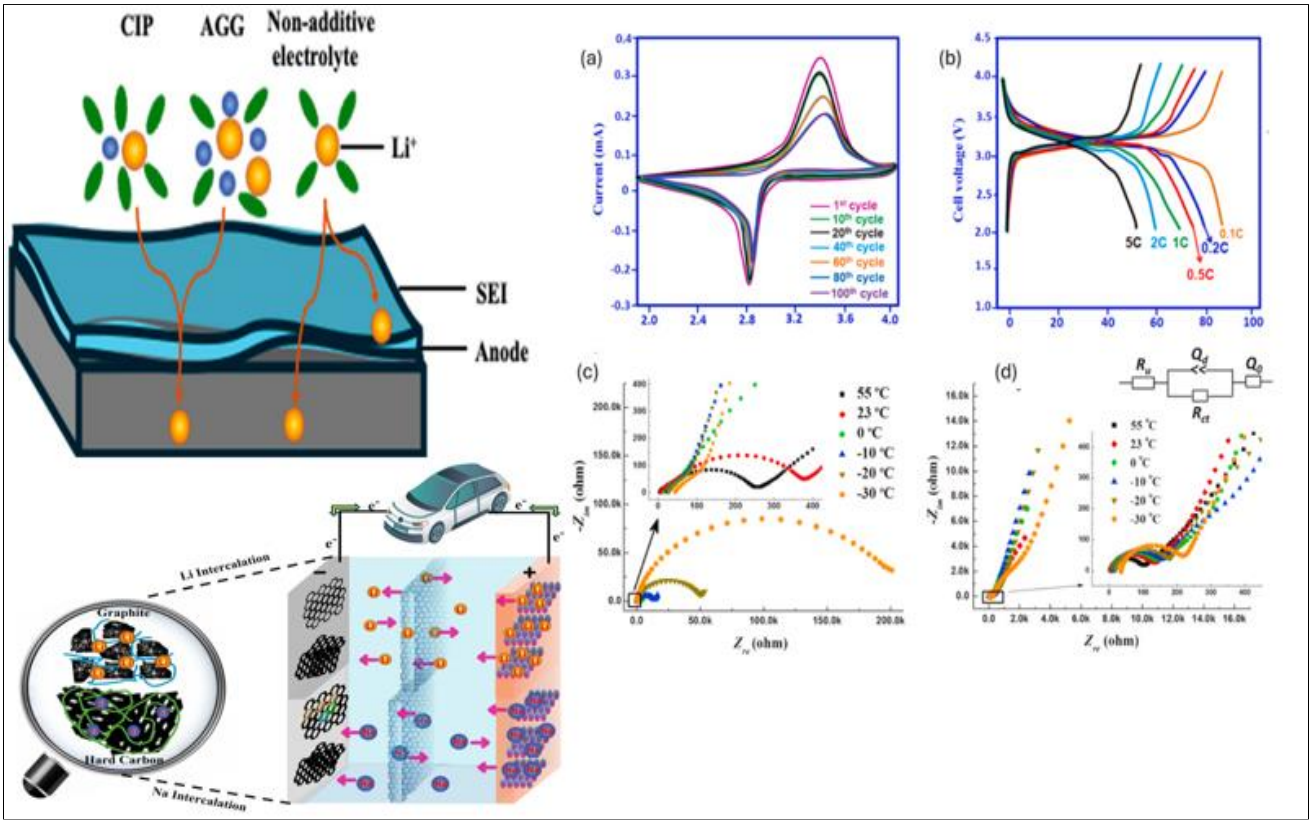


**Fig. 1: Electrochemical Fundamentals, Lithium vs Sodium – A Tale of Two Ions**

**Electrolyte Alchemy, Liquid, Solid, and Beyond**

Because they facilitate ion transit between electrodes, electrolytes are essential to electrochemical systems and control battery durability, performance, and safety (Xu *et al*., 2014). Because of their strong ionic conductivity and compatibility with a wide range of cathode and anode materials, conventional organic liquid electrolytes, typically made of lithium salts dissolved in carbonate solvents, have long been the industry standard. However, there are serious safety issues associated with their flammability, volatility, and thermal instability, particularly in harsh or high-temperature environments. Solid-state electrolytes (SSEs), a cutting-edge area of battery development, have attracted a lot of attention as a result. SSEs are perfect for high-energy-density applications of the future, such as electric cars and aerospace systems, because they completely stop leaks and significantly lower the risk of thermal runaway. Additionally, they make it possible to employ lithium metal anodes, which can greatly increase the capacity of energy storage (Guo *et al*., 2017). Their broad acceptance is nevertheless hampered by issues such as mechanical brittleness, low ionic conductivity at ambient temperature, and poor interfacial contact, despite their potential. In the meantime, new electrolyte chemistries are expanding the possibilities. Ionic liquids are appealing for high-temperature and high-voltage applications because of their remarkable electrochemical and thermal stability, which stems from their non-volatile and non-flammable nature. Gel polymer electrolytes combine the advantages of liquids and solids to create safer, more flexible structures with increased mechanical strength. Furthermore, flame-retardant electrolytes with cutting-edge additives are becoming more popular as a middle ground between improved safety and conventional performance. Thus, electrolyte design alchemy is changing from strictly functional to multifunctional systems, opening up hitherto unheard-of possibilities for energy storage technologies of the future (Zafar *et al*., 2025).

**Table 1: Electrolyte Alchemy: Liquid, Solid, and Beyond**

| Electrolyte Type | Composition & Structure | Key Advantages | Primary Limitations | Typical Applications |
|---|---|---|---|---|
| **Organic Liquid Electrolytes** | Lithium salt (e.g., $LiPF_6$) in carbonate solvents (e.g., EC, DMC) | High ionic conductivity; well-established; good electrode compatibility | Flammable; prone to leakage; unstable at high voltages | Lithium-ion batteries (consumer electronics, EVs) |
| **Solid-State Electrolytes (SSEs)** | Inorganic ceramics (e.g., LLZO, sulfides) or solid polymers (e.g., PEO-LiTFSI) | Non-flammable; prevents leakage; enables lithium metal anodes; higher energy density | Brittle structure; interfacial resistance; lower room-temp conductivity | Solid-state lithium batteries, aerospace, EVs |
| **Ionic Liquids** | Room-temperature molten salts (e.g., EMIM-TFSI) | Non-volatile; wide electrochemical window; high thermal stability | Expensive; lower ionic conductivity; sensitive to moisture | High-voltage and high-temperature battery systems |
| **Gel Polymer Electrolytes** | Liquid electrolyte entrapped in polymer matrix (e.g., PVDF-HFP + liquid electrolyte) | Flexible; safer than liquid; good mechanical stability; adaptable shapes | Lower conductivity than liquids; limited long-term stability | Wearable electronics, flexible batteries |
| **Flame-Retardant Electrolytes** | Organic solvents with flame-retardant additives (e.g., phosphate-based) | Enhanced thermal safety; improved fire resistance | Trade-off with ionic conductivity; chemical compatibility issues | High-safety lithium-ion batteries (grid storage, EVs) |

**Interface Engineering: The Battle of SEI and Interphases**

Particularly in lithium-ion and sodium-ion batteries, where the stability and nature of the interfacial layer have a major impact on cycle life, safety, and energy efficiency, solid-electrolyte interphase (SEI) formation continues to be one of the most important and intricate aspects of electrochemical cell performance (Hou *et al*., 2023). Due to the advantageous reductive breakdown of carbonate-based electrolytes, the SEI in lithium-ion systems spontaneously arises during the initial charging cycles and is often stable, producing a thin, passivating layer made up of organic species and inorganic salts (such as LiF and Li2CO3). Despite its fragility, this layer frequently facilitates long-term functioning. Addressing these differences calls for advanced interface engineering, especially at the nanoscale. Recent innovations include atomic layer deposition (ALD) and molecular layer deposition (MLD) of ultrathin coatings (e.g., Al2O3, TiO2, or organic-inorganic hybrids) on electrode surfaces to predefine SEI composition, suppress electrolyte decomposition, and accommodate volume changes during cycling (Zhao *et al*., 2021). Moreover, artificial intelligence and machine learning are transforming the design of interfaces by enabling the high-throughput screening of interfacial materials, predicting SEI growth dynamics, and optimizing electrolyte–electrode compatibility through data-driven models. AI-driven discovery platforms can now simulate and recommend nanocoating architectures with specific ionic conductivity, elasticity, and chemical stability tailored to Li+ or Na+ systems. As SEI evolution continues to dominate the performance frontier, synergizing interfacial chemistry, nanotechnology, and AI is redefining the battle of SEIs and interphases across next-generation battery chemistries (Zhang *et al*., 2024).

**Performance Metrics and Reliability Showdown**

Performance criteria, including cycle life, rate capability, and temperature stability, are the cornerstones for assessing dependability and economic viability in the quickly evolving field of energy storage technologies, especially lithium-ion and sodium-ion systems (Nekahi *et al*., 2024). For applications ranging from grid-scale storage to electric automobiles, a long cycle life guarantees that the battery will retain a high capacity across thousands of charge-discharge cycles, which directly affects the battery's sustainability and cost-effectiveness. For high-power applications, rate capability, which gauges a battery's capacity to give or take charge quickly, is essential. It affects responsiveness in renewable energy buffering and EV acceleration. Another important factor is temperature stability, since thermal runaway and capacity loss in harsh environments can seriously compromise long-term operation and safety. Robust electrode-electrolyte interfaces and sophisticated thermal management techniques are being developed to reduce deterioration at both high and low temperatures (Zhu *et al*., 2023). Enter the world of smart electrolytes and self-healing materials, which are pushing the limits of performance. By incorporating self-healing polymers into battery topologies, microcracks in electrodes can be automatically repaired, extending cycle life and reducing mechanical deterioration. Smart electrolytes, on the other hand, improve rate capability and heat resilience by suppressing dendritic formation and dynamically adjusting ionic conductivity. By introducing adaptive activity into previously passive materials, these next-generation technologies open up new possibilities for batteries to react intelligently to environmental variations, usage patterns, and stress. The combination of these technologies signifies a paradigm change toward robust, self-regulating electrochemical systems rather than merely a little improvement (Wang *et al*., 2025).

**Beyond the Cell, Pouch, Prismatic, and Flexible Configurations**

Innovation in form factor design has emerged as a major force behind the advancement of mechanical flexibility, energy density, and application versatility in the rapidly changing field of sodium-ion battery (SIB) technology (Wanison *et al*., 2024). In order to fulfill the demands of portable devices, electric vehicles, and future wearable systems, the industry is quickly moving toward more sophisticated configurations, such as pouch-type and flexible batteries, which have historically been dominated by cylindrical and prismatic formats. Pouch cells provide better packaging efficiency, lower weight, and a higher gravimetric energy density because they use laminated aluminum-plastic sheet enclosures rather than solid metal casings. Better thermal management and modular scalability are two benefits of prismatic cells, which are frequently utilized in automotive applications. Wearable and flexible sodium-ion devices, a popular trend that meets the increasing demand for energy storage systems that adapt to irregular surfaces or the human body, are the most revolutionary breakthrough, though (Ma *et al*., 2020). Stretchable, bendable, and even foldable battery designs are made possible by these next-generation topologies, which include flexible substrates, gel polymer electrolytes, and structurally malleable electrodes such carbon nanofiber mats or MXene-based composites. Their incorporation into smart fabrics, bio-integrated electronics, and health-monitoring wearables creates previously unheard-of opportunities in consumer and biomedical electronics. Additionally, performance stability under mechanical deformation and environmental exposure is ensured by moisture-resistant structures and sophisticated encapsulation techniques. An important turning point in the development of sodium-ion technology is the transition from traditional rigid cells to flexible form factors, which combine functionality, portability, and cutting-edge user experience (Deshmukh *et al*., 2015).

**Environmental and Economic Impact Analysis**

In terms of long-term sustainability, economic viability, and environmental impact, lithium and sodium are very different (Batuecas *et al*., 2024). Despite being essential for high-energy-density batteries, lithium extraction, especially from brine sources in South America, raises serious environmental issues. In already dry areas, water-intensive mining exacerbates water scarcity and disturbs delicate ecosystems, posing significant ethical and ecological issues. Furthermore, supply chain vulnerabilities and economic dependencies are brought about by the geopolitical concentration of lithium reserves, which are primarily found in the so-called "Lithium Triangle" (Chile, Argentina, Bolivia), as well as portions of China and Australia. On the other hand, sodium provides a more sustainable and regionally democratized option because it is the sixth most prevalent element in the Earth's crust and is found in large quantities in seawater (Thys *et al*., 2003). However, when it comes to energy density, sodium-ion batteries still fall short of their lithium-ion equivalents, which limits their usefulness in applications like electric vehicles that require small, high-capacity storage. Is sodium-ion technology the energy storage industry's green savior or just a niche candidate fit for low-cost and stationary storage applications? Proponents contend that sodium-ion batteries could transform sustainability by lowering prices and reducing resource strain for grid-scale storage, where weight and volume are less important factors. However, detractors highlight the relatively early commercialization stage and performance constraints, implying that sodium-ion may never become as widely used as lithium (Rudola *et al*., 2021).

**Table 2: Comparative Sustainability Analysis of Lithium vs Sodium for Energy Storage Applications**

| Aspect | Lithium | Sodium |
|---|---|---|
| **Abundance in Earth's Crust** | Relatively scarce (0.002–0.006 wt%) | Highly abundant (2.6 wt%) |
| **Sources** | Brine pools (South America), hard rock (Australia, China) | Seawater, rock salt, soda ash, industrial by-products |
| **Global Distribution** | Concentrated in limited regions (e.g., Lithium Triangle, Australia, China) | Widely distributed across continents, including oceanic availability |
| **Extraction Process** | Environmentally taxing; high water use, ecosystem disruption, chemical pollution | Comparatively low-impact; simpler chemical processes; less toxic waste generation |
| **Water Usage** | High (especially in brine extraction—up to 500,000 gallons per ton of lithium) | Minimal; standard industrial processes without extensive water dependency |
| **Carbon Footprint** | High due to mining, transportation, and chemical processing | Lower; uses existing salt and industrial waste streams |
| **Recyclability** | Growing but complex due to diverse battery chemistries | Easier pathways emerging due to fewer complex materials |
| **Toxicity and Environmental Risk** | Potential soil and water contamination; hazardous chemical handling | Relatively lower; less toxic materials involved |

| | | |
|---|---|---|
| **Production Cost** | High and volatile due to resource demand and extraction difficulty | Low and stable due to material abundance and low-cost processing |
| **Energy Density (Battery Output)** | High (150–250 Wh/kg) – suitable for EVs and portable electronics | Moderate (90–150 Wh/kg) – more suitable for stationary/grid-scale storage |
| **Market Maturity** | Advanced commercialization, vast infrastructure, robust supply chain | Emerging technology; limited industrial-scale deployment |
| **Geopolitical Sensitivity** | High – dominated by a few nations, risk of supply bottlenecks and price manipulation | Low – widely available, reduces geopolitical dependence |
| **Economic Scalability** | Economies of scale reached but at environmental trade-offs | High potential for cost-effective, decentralized energy storage solutions |
| **Suitability for Green Energy Grids** | Effective but environmentally constrained | Highly suitable due to sustainability and material availability |
| **Future Outlook** | Continued dominance with environmental reforms needed | Strong growth forecast for grid applications; potential disruptor in low-cost markets |

**Battery Safety and Thermal Runaway Prevention**

When implementing high-energy electrochemical storage systems, battery safety is still a top priority, especially given the extensive usage of lithium-ion (Li-ion) cells (Killer *et al*., 2020). Thermal runaway, a disastrous failure process brought on by excessive heat generation that can result in flames or explosions, is one of the most important problems. This condition frequently results from internal short circuits, overcharging, or mechanical damage in high-energy Li-ion cells, where exothermic reactions between the electrodes and electrolyte cause temperatures to rise quickly. Thermal gradients and isolated hotspots contribute to the propagation of failure, and the initiation of thermal runaway frequently occurs beyond 150°C, according to recent studies that have studied the thermal behavior of these cells with great spatial and temporal resolution (Jindal *et al*., 2019). Sodium-ion (Na-ion) batteries, which are frequently marketed as safer substitutes because of their more stable chemistry, are also being creatively redesigned to increase safety. These include the use of solid-state electrolytes that are resistant to thermal degradation, the creation of hard carbon anodes with regulated porosity to lessen dendritic growth, and the application of self-healing electrode coatings to prevent short circuits. Furthermore, AI-driven thermal diagnostics are being included in real-time battery management systems to anticipate and prevent dangerous situations in both Li-ion and Na-ion systems. Thus, the safety landscape of next-generation batteries is being reshaped by the combination of material breakthroughs and intelligent system design, guaranteeing improved heat resilience and wider use in consumer electronics, electric vehicles, and grid-scale storage (Hamdan *et al*., 2024).

**Real-World Deployment: Use Cases, Prototypes & Pilot Plants**

Lithium and sodium-ion batteries are quickly progressing from lab research to real-world application, showcasing their revolutionary potential in consumer electronics, electric vehicles (EVs), and grid storage (Abdolrasol *et al*., 2025). These developments are not only theoretical; full-scale case studies, operational prototypes, and pilot plants are being used to support them. Sodium-ion batteries provide affordable, thermally stable substitutes for lithium-based grid energy storage devices, making them ideal for extensive integration of renewable energy sources. With its sodium-ion battery, which was introduced in 2021 and has an energy density of 160 Wh/kg and can be charged to 80% capacity in 15 minutes, China's CATL has become a leader in this field. It is perfect for balancing intermittent renewable energy sources. The business has teamed up with automakers to incorporate the technology into next-generation EVs and has already started deploying it in electric two-wheelers (Nayak *et al*., 2023). Aiming for both grid and transportation applications, UK-based Faradion has created high-performance sodium-ion batteries with competitive energy densities and improved safety profiles. In Australia, Faradion's technology has been included into energy storage system prototypes, demonstrating practical scalability. Another significant Chinese player, HiNa Battery Technologies, has increased the production of sodium-ion batteries and started stationary storage trial projects with uses in telecom infrastructure and rural electricity. By providing safer, more plentiful, and more affordable alternatives for a variety of real-world scenarios, such as portable electronics, smart grids, and low-emission transportation options, emerging battery chemistries are actively influencing the future of energy storage and represent a paradigm shift (Nasri *et al*., 2025).

**AI, Machine Learning, and Computational Chemistry in Battery Design**

Computational chemistry, machine learning, and artificial intelligence (AI) are transforming battery design by speeding up the development, improvement, and use of cutting-edge energy storage technologies (Bajaj *et al*., 2025). Together, these technologies allow for a change from conventional trial-and-error experimentation to data-driven, predictive innovation. Researchers' methods for identifying and assessing promising options for lithium-ion and sodium-ion batteries are being revolutionized, particularly by the data-driven discovery of electrode materials. Scientists may make remarkably accurate predictions about electrochemical performance measures like capacity, stability, and voltage profiles by utilizing machine learning algorithms and high-throughput computational screening that have been trained on extensive databases of material attributes. The time and expense involved in creating next-generation electrodes are significantly decreased by this method. At the same time, atomic-level insights into ion transport, interfacial reactions, and structural transformations are provided by computational chemistry methods like density functional theory (DFT) and molecular dynamics simulations (Hao *et al*., 2023). These insights are crucial for creating materials with improved cycle life and safety. In addition to speeding up parameter adjustment, the use of AI in these simulations reveals previously unknown structure–property connections. Additionally, real-time lifecycle prediction and performance monitoring under a range of operating situations are made possible by the development of digital twins, which are virtual copies of actual battery systems. These digital models are effective tools for predicting failure modes, minimizing degradation, and optimizing charging processes because they are constantly learning from experimental and operational data. Thus, the combination of AI, ML, and computational chemistry offers a revolutionary route to the logical development of long-lasting, high-performing, and sustainable battery solutions for the clean energy of the future (Xu *et al*., 2023).

**Emerging Hybrid Systems and Dual-Ion Technologies**

The field of electrochemical energy storage is being redefined by emerging hybrid systems and dual-ion technologies, which combine the benefits of various chemistries in a way that overcomes their particular limits (Dou *et al*., 2021). Li-Na, Zn-Na, and Li-S hybrid systems are among the most promising designs; they provide increased energy density, longer cycle life, and cost-effectiveness for applications of the future. Li-Na hybrid systems combine the high energy density of lithium with the abundance and affordability of sodium to create reliable systems that can be used in both portable and grid-scale applications. These systems frequently combine a sodium-based cathode with a lithium-based anode, or vice versa, to provide thermal stability and adjustable electrochemical characteristics. Zn-Na hybrids combine the affordability and accessibility of sodium with the safety and environmental friendliness of zinc chemistry (Lv *et al*., 2024). Because of their environmental friendliness and non-flammable aqueous electrolytes, these systems are appealing for stationary storage. Although they need advancements like solid-state electrolytes and polysulfide-trapping techniques to reduce shuttle effects and increase lifetime, Li-S hybrid systems utilize the ultra-high theoretical capacity of sulfur and the proven lithium chemistry. Sodium-Ion Capacitors (NICs) are especially notable because they combine high energy density and high power capability, making them an essential link between batteries and supercapacitors. Utilizing a battery-type anode and a capacitor-type cathode (or the opposite), NICs have exceptional cycle stability, quick charge-discharge capability, and the possibility of low-cost, large-scale manufacturing. In industries like electric vehicles, renewable energy integration, and smart grid technologies that require both high performance and economical scalability, these hybrid devices are becoming more and more popular (Mwasilu *et al*., 2014).

**Policy, Recycling, and Circular Economy**

As the global demand for battery storage surges, the nexus of policy, recycling, and circular economy becomes increasingly pivotal in shaping the future of lithium and sodium-based electrochemical systems (Nekahi *et al*., 2024). Lithium's centrality in energy geopolitics has intensified due to the limited concentration of reserves in politically sensitive regions, such as the Lithium Triangle in South America and select deposits in China and Australia. This has triggered a wave of nationalistic policies, export controls, and supply chain security initiatives, prompting countries to diversify sources and explore alternatives like sodium-ion batteries, which rely on more abundant and geographically distributed resources. Sodium, often extracted from seawater or industrial byproducts, is emerging as a strategically valuable material due to its lower environmental footprint and reduced geopolitical tension. In this context, circular economy strategies, particularly closed-loop battery recycling, offer a critical buffer against resource scarcity and price volatility (Hagelüken *et al.,* 2022). Advanced mechanical, hydrometallurgical, and direct recycling methods are now being designed to recover valuable components like lithium, cobalt, nickel, and even sodium, minimizing the need for virgin mining. The *Spicy Spotlight* shines on closed-loop battery recycling and second-life applications, such as repurposing retired EV batteries for grid storage, telecom, or microgrid backup—extending their utility while reducing e-waste. Effective policy frameworks, including extended producer responsibility (EPR), eco-labeling, and recycling incentives, are vital to drive industrial compliance and innovation. Together, these interlocking domains create a resilient and sustainable materials ecosystem that underpins the future of clean energy technologies, reduces geopolitical dependencies, and aligns with global climate targets (Ibekwe *et al*., 2024).

**Future Forecast**

The competition between lithium-ion (Li-ion) and sodium-ion (Na-ion) batteries is anticipated to influence the energy landscape until 2035 as the world's drive for scalable and sustainable energy storage heats up (Titirici *et al*., 2024). According to predictive techno-economic models, Na-ion is set to make a big impact in cost-sensitive, large-scale energy storage systems (ESS), grid applications, and emerging economies, while Li-ion will continue to rule in high-performance applications like electric vehicles (EVs), consumer electronics, and aerospace. Although lithium's high cost, geographic scarcity, and supply chain weaknesses are expected to worsen over the next ten years, its better energy density and established infrastructure provide it a competitive edge in energy-dense situations. On the other hand, salt is perfect for fixed applications and mobility solutions where weight and volume limits are less important due to its abundance, cheaper raw material costs, and safer thermal stability. According to predictive modeling that takes into account life-cycle cost analysis, raw material forecasting, technological maturity indices, and policy incentives, Li-ion is still leading the EV market, but Na-ion may take over 30% of the stationary storage market by 2030, especially in Asia and Africa. But new developments like solid-state designs, hybrid Li-Na chemistries, and AI-optimized battery management systems could make it harder to distinguish between these technologies. As each technology carves out dominant niches suited to its distinct capabilities and techno-economic viability, the "ion war" may ultimately result in a functional coexistence rather than a single victor (Marsland *et al*., 1983).

## CONCLUSION

There has never been a more important moment for the direction of modern chemistry, particularly concerning energy technology, for our shared future. From revolutionary advancements in lithium and sodium-ion batteries to advances in hydrogen fuel cells, $CO_2$ conversion, and green catalysis, the field has progressed from small-scale enhancements to revolutionary discoveries. These developments represent a daring rethinking of how we capture, store, and use energy in addition to a deeper comprehension of atomic and molecular interactions. It becomes clear that there isn't a single, all-encompassing solution as we traverse the challenging landscape of energy sustainability. The real revolution, on the other hand, is turning out to be the strategic cohabitation of several chemistries that are suited to certain applications, resource availability, and geographic requirements. Our approach to energy design, manufacturing, and policy is changing as a result of the transition from technological competition to synergy. The true innovation is in maximizing the coexistence of lithium, sodium, hydrogen, and organic systems—integrating them where they work best and facilitating a decentralized, resilient, and fair energy landscape—instead of seeing them as competitors. In the end, designing a collaborative ecosystem that combines adaptability, scalability, and sustainability is more important than deciding on the greatest single course. The foundation for a cleaner and more flexible energy future is laid by the realization that coexistence may be the most radical innovation of all.

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