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Advanced Materials for Energy Storage: Batteries, Supercapacitors, and Beyond

Dr. Dhirendra Kumar
Assistant Professor,
Department of Chemistry,
Kashi Naresh University, Bhadohi
dhirendra08352@gmail.com

Abstract

As we work towards a decarbonised future, energy storage technologies will be vital. New and advanced materials are attracting attention as potential solutions to improve safety or performance beyond the limitations of conventional Li-ion batteries. Electrical energy storage systems are designed using materials and components such as active storage materials, conductive additives, supports, and coatings, which are critical to their architecture. Energy storage science and activity, therefore, centre on material design. The application range of energy storage materials has expanded to include Li-ion and post-Li batteries, supercapacitors, superconducting energy storage, and hybrid configurations. Materials must be optimised for specific technological applications. The essential performance parameters of energy storage systems are capacity, power, cycle life, safety, environmental footprint, and cost. All materials of interest must be explored and documented with specification ranges to enable quick assessment of new options and a focused search for them, to satisfy the emerging demand for energy storage.

Keywords: *Energy storage materials, Lithium-ion batteries, Supercapacitors, Solid-state electrolytes, Sodium-ion batteries, Pseudocapacitors, Nanostructured electrodes, Renewable energy integration.*

1. Introduction

Energy storage is a key technology that adapts electric systems and their present and future generation technologies (nuclear fission, renewable energy sources). Energy storage means that energy created when demand is low is either immediately converted into products, which are stored and then converted back into energy in a cycle, or stored in bulk and released to the grid when needed. According to Czagany and others in 2024, this creates a scenario that requires energy storage technologies to be adaptable for both grid-scale and consumer-level use, or somewhere in between. Advances in consumer electronics have made portable energy storage devices, including batteries and supercapacitors, among the most important technological fields. According to Balasubramaniam et al. (2020), this review describes the technology and materials used in these systems. Furthermore, it summarises materials research activities on various energy-storage materials.

2. Fundamentals of Energy Storage Materials

Energy storage is modern technology's key element because it makes electrical power produced by renewable resources available by overcoming the 'down-times' intrinsic to electrical systems, as in any conventional electrical system. Nowadays, energy storage accounts for a sizeable share of renewable energy (RE) developed globally. The world is witnessing a shift toward Radical Energy (RE) technologies, including wind, solar, wave, biomass, hydro, geothermal, fossil fuels, and nuclear. A key requirement for enabling large-scale renewable energy adoption into society's energy chain is the establishment of highly efficient, fast energy storage technologies. An energy storage system can store excess energy from RE technology and utilise it hours, days, or weeks later (Balasubramaniam et al., 2020).

Energy storage systems can be classified as electrochemical, mechanical, thermal and electrostatic storage (Kamali-Heidari et al., 2018). Devices that store energy as electrochemical cells could include batteries and fuel cells. Any battery system consists of four basic components: anode, cathode, electrolyte and separator membrane. Lithium-ion battery technology is primarily used for energy storage via the insertion and extraction of lithium ions. It takes place during charge/discharge cycles. Lithium-ion battery technology is also used in electric and hybrid electric vehicles. The performance is represented with a two-dimensional system: energy and power densities (Czagany et al., 2024). Fuel cells have the highest energy density among the four groups, but their safety challenges and operational constraints limit their use. An ideal battery system should be low-cost to manufacture, have a long service life, be safe, and have high energy density.

2.1. Electrochemical Principles

Energy storage via electrochemical means is important in the transition to sustainable energy systems. Mechanisms of storing electrochemical energy include batteries, electrochemical capacitors, and fuel cells. A battery is made of an anode, a cathode, a separator, and an electrolyte. When rechargeable batteries are charged and discharged, ions move through an electrolyte and conductive additives (Kamali-Heidari et al., 2018). Lithium-ion batteries use lithium ions, which intercalate and deintercalate between the anode and cathode during discharge and charge, respectively. The electrochemical storage device's performance depends on its chemistry and the material and architecture choices made for the device.

The standard performance metrics at the device level include gravimetric energy density, gravimetric power density, cycle stability, and safety. Gravimetric energy density is the amount of electrochemical energy stored per unit mass (Wh·kg–1). Gravimetric power density is the speed with which this energy can be delivered (W·kg–1). According to Mukherjee et al. (2018), cycle stability refers to a device's ability to maintain its performance over cycling. For the materials under consideration, these specifications are too vague because they do not distinguish between materials that deliver energy through a fast kinetic process within seconds and those that do so via a diffusion-limited process that takes much longer (Balasubramaniam et al., 2020). To differentiate energy-storage technologies, the cycle life of a battery is defined as the number of charge–discharge cycles before the cell's capacity falls below 80%. The supercapacitor life is defined as the number of cycles required for the system to reach a specified capacitance retention level, e.g., 80%.

2.2. Material Classes and Architectures

Energy storage materials can be classified by structure into bulk, nanoscale, composite, thin-film, and 2D materials (J. Osiak et al., 2018). Bulk systems, which remain commonplace, have relatively long pathways for ion diffusion and electron transport. The process of nanostructuring markedly reduces these distances and enhances kinetic movement, permitting a range of phase-change, conversion, and alloying electrode materials to be employed. Composites allow the combination of diverse active materials. Active materials can also be mixed with conducting additives and binders to allow charge transport. Nanostructuring of mixed-phase systems can produce hybrid materials that employ multiple mechanisms. Thin-film- and 2D material-based design offers the advantages of nanoscale dimensions and high-capacity active materials. Meanwhile, the large interface area reduces the volume change of active materials and shortens the ionic diffusion distance.

3. Lithium-Based Batteries

Emerging from early nickel–cadmium systems and evolving through today's lithium-ion technology, lithium storage batteries deliver electrochemical energy through intercalation, conversion or alloying mechanisms in several applications. During discharge, electrodes employ a common-ion-drainage principle, with ions moving from the anode via a common electrolyte to the cathode. The two interfaces, anode–electrolyte and cathode–electrolyte, are concurrent yet independent, each a single electrochemical system governed by the conventional energy–power trade-off. The studies focusing on lithium storage materials address performance, safety, lifespan, cost, and material sustainability (J. Osiak et al., 2018); dimensionality control; surface modification; composite formation and hetero-architectures (Mukherjee et al., 2018) and morphology design (Chen, 2013).

3.1. Lithium-Ion Technologies

Lithium-ion batteries work by the movement of lithium ions through the electrolyte and electrons in the external circuit. Carriers exhibit an explicit reaction mechanism for entering and leaving the electrodes. The anode's lithium reduction is coupled to the cathode's oxidation, and vice versa. All the cell chemistries presently in commercial use exhibit this coupling (J. Osiak et al., 2018). Carbonaceous compounds or silicon-based composites are the most common anode materials. According to Chen (2013), cathode materials can be grouped into lithium metal oxides, lithium metal phosphates, and lithium transition metal sulfides. The energy density is closely linked to the material’s theoretical capacity and the average cell voltage.

The chemical composition of cell components affects many performance metrics, such as safety, life, charge/discharge rate, temperature window, and component compatibility, for any target application. Insights from the lithium-ion battery cell literature on mechanisms of performance mitigation and design strategies at the cell level.

3.2. Lithium-Sulfur and Lithium-Mulivalent Systems

The focus on Lithium-sulfur and lithium multivalent systems is growing because they have high energy density and are comparatively low-cost compared with conventional lithium-ion systems (Kien Juen Ting et al., 2022). The lithium-sulfur cathodes show a theoretical sulfur utilisation near 80%, and the storage of 7.5 Li per S. Problems related to such cathodes involve the loss of active sulfur and side reactions with the anode due to the soluble polysulfides’ shuttling effect, and volume expansion of S/Li2S upon cycling. It is, therefore, of significant interest to create lithium-sulfide systems in which S is fully reduced to Li2S and the soluble polysulfide formation pathway is avoided. Nonetheless, the high first-charge overpotential due to the insulating nature of Li2S and the demanding conditions of solid-state reaction are major challenges. The cycling performance is significantly enhanced when Li2S discharge is followed by Li2S2 reoxidation, compared with either full reduction and reoxidation of Li2S or direct S oxidation.

Lithium–magnesium, lithium–calcium, and lithium–aluminium batteries are emerging lithium multivalent systems. These systems are attractive due to their potentially high theoretical capacities, which can exceed 8000 mAh per cell depending on the specific chemistry and anode material. The enhanced capacity arises from multivalent ion charge transfer, where ions such as Mg^{2+}, Ca^{2+}, or Al^{3+} can transfer more than one electron per ion during electrochemical reactions.

However, the practical implementation of these systems is hindered by sluggish ion diffusion, strong electrostatic interactions, and the formation of passivation layers. Solid–electrolyte interphase (SEI) formation and stability play a crucial role in determining battery performance. Effective interface engineering and electrolyte design are therefore essential to improve reversibility, cycling stability, and overall efficiency of multivalent battery systems.

3.3. Solid-State Electrolytes and Interfaces

Solid electrolytes are believed to enable all-solid-state lithium-based batteries, potentially offering a wider operating temperature window, longer cycle life, enhanced safety, and higher energy density than conventional liquid electrolyte systems (Falco et al., 2019). Even though they are advantageous, their performance is lower than that of liquid-based batteries due to the complexity of their interfacial chemistry. To realise high energy density, compatible materials must be judiciously chosen to minimise parasitic reactions during cycling and stress development. Those strategies typically involve composite and multilayer designs that allow for the independent tailoring of the component characteristics in the electrode, electrolyte and solid electrolyte throughout the cell. The microstructure of solid composites and single-component electrolytes will affect transport properties in general and device performance in particular. For instance, particle morphology, size, and fabrication protocols significantly affect performance. Techniques that are multivariate, in situ, and/or real-time offer valuable avenues for understanding the process-microstructure-transport-property relationships.

The properties of solid electrolyte/electrode interfaces will significantly affect the efficiency of all-solid-state lithium batteries. In Zhu's (2018) paper, the author indicates that performance is severely limited by high interfacial resistance. This often leads to interphase formation, degradation, and low ionic conductivity. Since it is challenging to probe buried interfaces experimentally, computational modelling approaches such as first-principles calculations and molecular dynamics simulations can provide atomic-level insights into them. It is essential to understand the intrinsic electrochemical stability windows of the solid electrolytes LGPS and LLZO to avert interphase formation, which can lead to excessive resistance and impair overall battery performance.

4. Beyond Lithium: Alternative Chemistries

Lithium-ion batteries have become the most popular technology for electrochemical energy storage owing to their high energy density and long cycle life. Sustainability and the security of lithium supply chains are growing concerns as the LIB market continues to expand. Various research groups have tested alternative battery chemistries based on abundant and harmless materials to LIBs, such as sodium, potassium, magnesium, aluminium, zinc, and iron, for different applications (Sadd, 2019), which are high on the agenda. Sodium and magnesium batteries are among the most widely studied alternatives to lithium batteries; accordingly, their chemistries are presented in Sections 4.1 and 4.2, respectively. Aluminium- and zinc-ion batteries are also promising candidates for large-scale stationary storage applications (Leisegang et al., 2019)—section 4.3 analyses multivalent ions and other charge carriers beyond lithium, which are gaining popularity in batteries.

4.1. Sodium and Magnesium Batteries

Sodium and magnesium batteries offer promising energy storage solutions, as sodium is plentiful; moreover, magnesium is less hazardous to transport and handle than lithium. Researchers have focused on developing suitable electrode materials and electrolytes for better performance. Sodium-ion batteries are potential competitors to lithium-ion batteries because of sodium's abundance and cost advantages. Developments include high-capacity anodes made from tin, antimony, and transition-metal phosphides with various nanostructures, enhancing capacity and cycling stability. Electrolyte formulations containing carbonate and fluoroethylene carbonate improve electrode stability. Current research seeks to enhance the effectiveness of the polysulphides and sulphides conversion mechanism in sodium-based sulphur batteries for large-scale energy storage (Wang et al., 2019).

Magnesium batteries, which are cheaper and more abundant than lithium-ion batteries, hold the potential to become the future battery technology. Batteries store energy from intermittent renewable sources. Different energy storage systems have various capabilities that suit different applications, such as portable devices and grid storage. Battery technologies for electric vehicles are mostly concerned with volumetric capacity and safety. As a result, extensive research has been conducted on high-capacity metal-anode batteries, particularly magnesium (Carol Miller, 2015).

4.2. Zinc and Aluminum Batteries

Zinc (Zn) and aluminium (Al) batteries offer two alternatives to lithium-based electricity storage. The storage solutions depend on the respective Zn^{2+} and Al^{3+} ions. Al is lighter than Li (25% lighter) and has a lower energy density. However, the systems cannot yet compete with Li in terms of reversibility and cycle life. Other than that, Al electrodes can get high rates, much better than current Li systems. Research is also underway to find suitable electrolytes and alternative inactive materials to increase energy density. (Leisegang et al., 2019)

Al and Zn batteries must address several challenges to become commercially viable. Al can store 3 times as much charge (3e) as Zn (2e) for the same energy. Currently, existing storage materials cannot utilise 3e yet; either their packing is too compact (theoretical density too small for 3e) or too dispersed (energy density limited by packing size). The response is often only pseudo-3e, but still much more attractive than Zn. However, the problems remain to be solved urgently. There is an urgent need for effective prevention of the irreversible side reaction in rechargeable Zn batteries. Al tackles the cycle life from a distinct angle (Schötz et al., 2017).

4.3. Multivalent and Beyond-Lithium Concepts

The sodium-ion battery technologies are the most advanced after lithium-ion. "Beyond sodium, magnesium-ion systems are emerging as a post-lithium contender". The two chemistries use divalent ions, so there is a softer ion–ion interaction in the electrolyte with a larger crystal, which mitigates energy density. In addition, both chemistries exhibit limited power densities due to their low diffusion coefficients in solid electrodes. A battery design with a single component is simple, but it severely limits materials to periodic table trends.

Aside from sodium and magnesium, this innovation enables the use of multivalent systems based on zinc, aluminium, calcium and/or other trivalent and higher systems. Systems of several zinc, aluminium, or calcium posts, lithium, or their combinations, based on single-component cell designs, are still under consideration. Technologies discussed in this white paper are not fully explored or optimised; thus, their performance metrics, barriers to implementation, and avenues for investigation are not readily identifiable (Chen et al., 2016).

5. Superconducting and Pseudocapacitive Energy Storage

Supercapacitors, also known as electric double-layer capacitors (EDLCs), are positioned between batteries and conventional capacitors. They feature excellent cycling stability, fast charge/discharge rates and high power density. Power delivery continues to matter as much as energy storage; in small energy storage devices (ESSs), consumer electronics, electric vehicles, and renewables, batteries are still ahead on energy density, whereas the much shorter charging times of supercapacitors can be exploited in hybrid systems such as ultrabatteries and supercapatteries. According to researchers such as Czagany et al. (2024), supercapacitors are generally considered to store energy not through a Faradaic redox reaction but through the non-Faradaic formation of an electric double layer at the electrode-electrolyte interface. At highly porous carbon electrodes, which maximise the effective surface area, the capacitance is mainly determined by the pore size distribution – from sub-1-nm pores with capacitance of 2–5 F/cm2 to hundreds-of-nm ones. However, the associated energy density remains lower than that of batteries.

Pseudocapacitors exhibit superior capacitance and energy characteristics compared to conventional supercapacitors. This is due to the rapid surface Faradaic processes occurring at the electrode–electrolyte interface. These processes are characterised by fast charge-transfer electron transfer reactions along with ionic coupling (Guan et al., 2016). The presence of charge storage at other sites in the bulk of the material can introduce a different time scale. Pseudocapacitive intercalation and battery-type conversion processes are routinely much slower than ultra-fast surface electron transfer. Hybrid devices may thus be configured with materials with surface and bulk processes to decouple energy and power – these combinations tend to improve stability and lifetime. Meeting the above criteria and remaining stable is a constant problem. Nanostructured electrodes create a highly effective surface area (100-500 cm2/mg) and low diffusion length (< 10 nm) in a single structure, enhancing performance due to surface and bulk processes (Balasubramaniam et al., 2020).

5.1. Electric Double-Layer Capacitors

Electric double-layer capacitors (EDLCs), colloquially known as supercapacitors, are energy storage devices that can deliver high power density and long cycle life. Charge separation at the electrodes/electrolyte interface stores energy. This is often referred to as symmetric electrodes with a non-redox-active, neutral electrolyte. Pore structure optimisation and other design principles can improve overall performance by accelerating ion diffusion and enabling high-rate operation (Nee Yeo, 2011). Endurance-Level Charging Cells are specifically designed for applications that require both rapid charging and discharging. They offer a sustainable solution for storing electrical energy.

Essentially, the capacitance of EDLCs relies predominantly on the spontaneous formation of the electric double layer (EDL) at the electrode surface upon application of the potential. The polarisation of charge carriers in the electrolyte and the electrode surface area, the pore-size distribution, and the shape characterise the EDL. However, increasing surface area alone does not ensure maximised energy density per volume. To overcome this trade-off and optimise EDL capacitance, the electrode structure and electrolyte concentration should be tuned (Bo et al., 2018). Improvement depends on maximising quantum capacitance, which generates an additional layer of charge carriers when it equals the EDL capacitance. This allows the charge-discharge rate to reach a peak. This principle and materials properties may thus be understood quantitatively to develop optimal capacitors.

The principles of energy storage from an electrochemical perspective are quite similar to those of the storage mechanism. Thus, they are equally important. The fundamental system that describes charge evolution in an individual energy-storage cell can be used to introduce the governing concepts of capacity, voltage, and rate capability.

5.2. Pseudocapacitors and Hybrid Devices

Electric double-layer capacitors (EDLCs), which rely on interfacial charge separation at the interface between a porous carbon electrode and an electrolyte, can achieve high power density and cyclability. More recent pseudocapacitors do indeed achieve even higher charge storage density by electroadsorbing charge carriers via fast, reversible surface valence changes; they can thus use transition-metal and conducting-polymer-oxide materials. Hybrid devices that incorporate electrochemical double-layer capacitors (EDLCs) possess fast charge–discharge kinetics and a higher electrochemical potential due to high-capacity battery electrodes. Ceramic and nanostructured materials are often used to enhance ion accessibility in energy storage structures (such as electrodes).

In contrast to adsorption- and diffusion-controlled processes, metal oxides are integrated into the supercapacitor to enhance the working voltage via metal redox faradaic charge storage (pseudocapacitance). Energy storage in some pseudocapacitors is achieved electrochemically via transition metal oxides such as RuO_2, MnO_2, Co_3O_4, Fe_3O_4, and NiO, as well as conducting polymer electrolytes, rather than through simple double-layer mechanisms. The electrode–electrolyte interface experiences these effects as electroactive species cross the EDL, after which they undergo redox reactions. Despite the availability of materials with high double-layer capacitance, they do not readily integrate with faradaic charge–storage processes, which have much higher ramp rates. As a result, coprecipitated MnO_2 has been coupled with carbon to manufacture supercapacitors.

The design of structures to promote optimal pseudocapacitance is still in its infancy compared to all other classes of porous materials. A very large surface area and porous structure with sufficient accessibility for the charge carriers involved in the storing process are basic considerations. Purposeful initial design selection of pore configuration and size distribution facilitates the choice of dielectric for a suitable design of pore structure for optimum suppression of parasitic …√ current components. In addition to optimising size and performance, a Raman-processing window and pore architecture may also be influential.

5.3. Nanostructured Electrode Architectures

Electrode performance determines the overall efficiency of energy storage devices. Analysis of the structure, properties, and performance indicates that performance can be improved by increasing surface area, shortening diffusion pathways, and maintaining mechanical robustness. Nanostructured architectures satisfy these requirements but impose additional restrictions on material design, especially for electrodes that undergo large volume changes.

Architectures such as hollow, porous, or nanosheet structures address the conflicting requirements of electrochemical energy storage devices (Calcagno, 2020). Electrode frameworks with mesoporosity increase the charge storage in the electric double layer and promote rapid ion transport through long diffusion paths. 3D scaffolds with low density provide a nanostructured support that facilitates the deposition of thin films on surfaces and in confined spaces. The need for extensive pre-evaluation across numerous compositions is reduced when nanostructured materials are designed to exhibit electrochemical behaviour similar to that of the corresponding bulk materials (Qiu et al., 2024). An electrode made of a 3D-printed conducting polymer can enable flexible supercapacitors to achieve high capacitance. Microminiaturized honeycomb monoliths with ultrathin nanoscaffolds yield a micro-supercapacitor with high energy and power density. Concepts of advanced materials design and manufacturing techniques, as well as new pathways for electrochemical energy storage, are essential to meeting energy demand and advancing R&D efforts.

6. Electrode Materials Design and Engineering

A large number of studies focus on the design and engineering of electrode materials for energy storage devices. For anodes, silicides and transition-metal phosphides are investigated for lithium storage. The lithium storage capacity per silicon atom is over 10 times that of graphite in lithium-ion batteries. However, the material's large volume change during cycling induces stress and cracking, which drastically reduces capacity. Different strategies have been adopted to reduce such deterioration: (i) Alloying anode materials like Sn or P, which are characterised by lithiation that produces mechanical expansion coupling of two or more times lower than that of Si and provides high capacity nevertheless. Intercalation compounds display basic diffusion processes. For example, TiS_2 or niobium oxide. Anode materials that are barely affected by large-scale insertion behaviour. Such as SiO_2, nanostructured zero-strain TiO_2, and ZnO.

The main cathode components in lithium-ion batteries are layered oxides, such as $LiCoO_2$, and complex oxides, such as spinels. The performance of smart coatings is enhanced by Li-rich layered oxides, such as Li_2VO_2F, which are designed to achieve long lifetimes. Co-free layered oxide alternatives and layered oxides compatible with aqueous electrolytes are under investigation (Czagany et al., 2024). The architecture of complex oxides incorporates additional structural dimensions that enable operation above the 4 V limit. Further utilities include redox activity at ambient conditions, together opening avenues for hybrid aqueous devices.

Lithium sulphur batteries, which combine an elemental sulphur cathode and a lithium anode, theoretically offer the highest gravimetric energy density available. The selected conductive material alters sulfur loading and cathodic electroactivity. Additionally, carbon black, CNTs, and graphene are among the few materials that can achieve a high degree of sulfuration while remaining conductive. The study of polymer electrolytes might help to suppress polysulfide dissolution (Ramachandran et al., 2019).

6.1. Anode Materials

For their high theoretical capacities (e.g., 4200 mAh/g for Si), alloy materials (e.g., Si, Ge, SiGe) have been extensively studied as anode candidates. Even with a volume change of 60-70% during cycling, it undergoes lithiation and delithiation at low voltages, making these Si-benched materials candidates for broken-Se or film devices (Mukherjee et al., 2018). Nonetheless, most research has focused on Si-based composites to suppress large volume expansion and maintain electrical connectivity, thereby enabling high capacity. Water vapour in the atmosphere can make highly reactive materials even more reactive (Kamali-Heidari et al., 2018).

Materials with high capacity show very low diffusivity. Alternatively, materials with a high diffusion coefficient exhibit very low capacity either because their atomic arrangement is already saturated, or they show very low voltage. As a result, we must take into account that the large electrode structure or many tightly bound materials with electrolyte seep into that material, allowing rapid Li diffusion to overcome the limited speed.

6.2. Cathode Materials

Battery cathodes can be classified into various categories based on their crystal structure, charge-storage mechanism, and other properties. These include layered oxides (or intercalation compounds), spinel oxides, polyanionic compounds, and conversion materials. Lithium cobalt oxide is one of the most commercially successful layered oxide cathode materials. These materials also include lithium nickel cobalt oxide and lithium nickel manganese oxide, among others. The oversized first irreversible capacity and safety issues arising from unexpected phase transformations during cycling call into question the commercial application of Lithium Cobalt Oxide (LiCoO2). Thus, ecological issues arise from the utilisation of such materials.

A suitable alternative to layered cathode materials, due to its environmental benignity and low cost, has been developed: Spinel (e.g., $LiMn_2O_4$). Unfortunately, the battery performance is poor. Researchers have created many new polyanionic materials, including lithium iron phosphate ($LiFePO_4$), lithium manganese phosphate ($LiMnPO_4$), lithium vanadium phosphate ($LiVPO_4F$), lithium titanium phosphate ($LiTi_2(PO_4)_3$), and others, to improve thermal stability further, reduce explosion risk and enhance cycle life of battery systems. Due to their distinctive three-dimensional structure and enhanced structural and thermal stability during charge/discharge cycling, these materials have attracted considerable attention. However, it limits their fast-charging and long-cycle capability due to the low conductivity of these compounds. In the list of materials, lithium iron phosphate ($LiFePO_4$) is a potential next-generation cathode material due to its affordable cost.

Therefore, it is required to improve the conductivity of $LiFePO_4$.

6.3. Protective Coatings and Interface Stabilisation

The lifetimes of batteries and supercapacitors are enhanced by techniques that stabilise interfaces and provide protective coatings. The manufacture of high-performance coated and stabilised magnetic nanomaterials is an area that attracts increasing attention, as their physical and structural properties strongly affect overall performance and safety (Kim et al., 2014). Just like interface stabilisation techniques dynamically alter interface properties during operation to improve life and reduce costs.

7. Electrolyte Developments and Interfacial Chemistry

In rechargeable metal batteries, the discovery of next-generation electrolytes and interfacial materials across a range of electrochemical systems is gaining focus to prevent deactivation, enhance battery safety and stability, and enable fast ion transport (Czagany et al., 2024). Liquid, solid-state, and gel-like electrolytes are suitable among them. Liquid electrolyte formulations are often used in organic solvent formulations, but non-aqueous lithium-ion batteries are excluded due to safety concerns. Consequently, attention has recently shifted to solid-state electrolytes (SSEs) to overcome flammability issues, safety hazards, and operational stability challenges, while maintaining low interfacial resistance. Polymer–ceramic composite-type solid electrolytes are some of the different types of SSEs. It is anticipated that a gel-like electrolyte will combine the advantages of both liquid and solid electrolytes. Furthermore, when screening frameworks formulated with ionic liquids, candidate pools for room-temperature operation are expected to be more extensive.

The kinetics of interfacial charge transfer at the electrolyte/electrode interfaces and the overall stability of the electrodes remain crucial. When the electrolyte and electrode pairs are matched, they can undergo more electrochemical reactions and decompose, giving rise to interphase layer(s) such as a solid electrolyte interphase (SEI) or cathode electrolyte interphase (CEI). The presence of these interphase layers severely limits the battery lifetime. It is essential to understand the formation and further evolution of these interphase films under operating conditions and cycles to ensure battery youth. Finally, supercapacitors are exceptional energy storage devices that operate via a distinct charge-storage mechanism and chemistry in an electrolyte. To illustrate, the electric-double-layer mechanism is less reliant on the solvent molecule, whereas supercapacitors and pseudo-capacitance-based supercapacitors are severely limited. To enhance future working potential, further investigation of suitable electrolyte systems is needed.

7.1. Liquid, Solid, and Gel Electrolytes

For conducting ion-solvent mixtures, liquid electrolytes based on organic solvents with high dielectric constants (such as ethylene carbonate) are generally employed. Nevertheless, such liquids are highly flammable and can leak, causing short circuits and thermal runaway. These also allow low-voltage cells (which are no longer used in high-energy compositions), but cannot be used at the supercapacitor voltages (where they would decompose and generate gaseous products). The performance of supercapacitors can benefit from versatile, non-flammable, non-leakable ionic-liquid electrolytes with high voltage (Pan et al., 2020). A potentially attractive feature of these cryotropic organic gels is the use of ionic liquid mixtures solvated in regular organic solvents. When applied to appropri-ate substrates, such formulations can enhance conductivity, lubricity, and electric double-layer capacitance. This has positioned this 20-year-old class of materials, which still covers an impressive operational temperature range from −140 to +300 °C, at the forefront of current supercapacitor efforts. In addition, they pave the way for novel science and technology, making possible an envisaged paradigmatic shift from enabling electricity as a burn-and-use / once-through commodity to a reusable, transportable and equitable resource (Peng et al.,2016).

7.2. Interfacial Charge Transfer and Stability

The interface between the electrode material and electrolyte determines the charge transfer, device functionality, and stability. The development of solid-electrolyte interphases (SEIs) on anodes, lithium metal anodes, and other protective and passivating layers on high-voltage electrodes helps improve cycle life and safety by curbing electrolyte decomposition, limiting dendrite growth, and minimising side reactions (Davies, 2018). In recessed geometries, charge-transfer dynamics can grow dominated by a few crystallographic planes, spatially decoupling charge transport and phase conversion.

7.3. Safety and Thermal Management Considerations

Energy storage devices store and deliver electrical energy through reversible electrochemical processes. The conversion of energy at the electrode–electrolyte interface through electrochemical reactions facilitates the exchange of ions and electrons. The electroactive solid-electrolyte interface exhibits rapid electron-transfer kinetics and ionic and atomic gas diffusion across solid-gas interfaces. Components that provide charge transfer, heating, and/or thermal insulation can have high ionic and electronic conductivity. These components inhibit gas permeation, reduce corrosion and prevent any liquid electrolyte loss during phase transitions. EDL supercapacitors rely entirely on surface charges stored at the EDL, whereas pseudocapacitors can store surface charges and undergo fast bulk redox reactions. Classification based on the cation functionality of cation-exchange-grafted (CEG) layers in ion-conductive membranes exhibits processes similar to those in natural systems. Stability, simple design, free-standing and low-cost electrodes are lacking in supercapacitor and/or pseudocapacitor development.

Investigation into energy-storage materials, such as batteries and capacitors, for electric vehicles, home energy-storage systems, and large grid stabilisers is still needed regarding self-heating. In conjunction with the development of complex devices, standard rectangular pouch cells may also benefit from controlled self-heating analysis of solid-state lithium-ion batteries. Thermal-management materials and technologies, plus exothermic additives and insulating separators that do not electrochemically react, aid heat retention.

8. Advanced Characterisation and Modelling

Advanced characterisation and modelling of supercapacitors encompasses the synthesis of porous Carbon nanosheets, including graphene and carbon nanotube composites, as well as other types of carbon, and the assessment of ionic liquids and ionic-liquid-based non-aqueous electrolyte systems. Advances in Na-ion capacitors, inorganic and organic electrolyte systems, and the effects of solvents on ion adsorption are key. The performance and flexibility of the device can be improved by using materials such as nanocarbon-based flexible supercapacitors, 2D wearables, quasi-solid-state electrolytes, and solid polymer electrolytes. Structural supercapacitors incorporating aligned, discontinuous carbon fibres with solid polymer electrolytes, and their application in wearable devices, are emerging advanced technologies (Czagany et al., 2024).

It is essential to understand the materials and processes for advancing energy storage. A polymer nanofiber is produced by electrospinning under high voltage, and molecular dynamics simulations are used under flow conditions to study the spatial distribution of nanoparticles in a polymer blend and to model the electrospinning process. Simulations of cylindrical confinement with decreasing diameters mimic electrospinning and show that morphology depends on deformation and self-assembly timescales. Models that include reaction, mass transport, adsorption, and nucleation are used to study the lithium–sulfur battery electrochemistry. These models help elucidate challenges, including polysulfide crossover and volume changes, identify that an inadequate polysulfide mass transport is a major failure mechanism, and that adsorptive materials can enhance performance by altering lithium sulfide deposition. Varying end-of-discharge failure mechanisms result from different cathode processing techniques.

8.1. In Situ and Operando Techniques

In situ and operando techniques have enabled characterisation of energy storage systems under operando electrochemical cycling conditions, including structural, chemical, and electrochemical analyses. Because traditional ex situ methods do not capture charge- and discharge-transient phenomena, the mechanisms at play remain poorly understood (Stangl et al., 2020). Techniques that collect data without removing electrodes from installed cells are called in situ. In operando techniques, data collected during material cycling are referred to as operando data. Various operando and in situ techniques using probes such as X-rays, visible and infrared light, and low-frequency radio waves have been employed across the energy storage landscape (Grant & O'Dwyer, 2022). Equipment techniques are components of laboratory apparatus widely used by the materials community.

8.2. Multiscale Modelling and Simulation

To design new energy storage systems, we need multiscale modelling and simulation to understand how atomistic properties and processes govern electrochemical performance at the device scale (Datta, 2023). To design materials successfully, we must understand how they couple over many different time and length scales. For example, atomistic phenomena underlie the macroscopic electrochemical response in a galvanostatic discharge. However, continuum modelling does not provide a framework for informing an atomic-scale strategy to improve performance (Shebert, 2019). Multiscale modelling is thus crucial in materials discovery for energy storage, albeit challenging.

8.3. Data-Driven Materials Discovery

The ongoing paradigm shift in the discovery and optimisation of materials is accelerating the development of advanced energy-storage systems (Alberi & Gregoire, 2019). The use of data and informatics, especially high-throughput screening and machine learning, is gaining popularity in materials research. The possibilities for searching the vast and diverse chemical-structure space and for multiple-step synthetic processes are growing. A generic crystal-screening procedure is applied to a lithium-silicon system to investigate the method's capabilities and limitations.

9. System-Level Integration and Applications

The energy storage requirements of portable and wearable electronics, electric mobility systems, grid storage systems and renewable energy systems are challenging. Mobile and wearable gadgets need compact, lightweight, thin, low-cost energy storage with energy densities of 5–15 Wh kg−1 and power densities of 500–1000 W kg−1. The target specifications are to maintain >80% capacity after 500 cycles and to meet maintenance requirements under either ambient or varying-temperature conditions (Czagany et al., 2024). An energy density of more than 200 Wh kg−1 in electric vehicles enables a range of 400 km. The life of the cycle was set at over 3000 cycles, and the total cost was under €300 per vehicle. In a grid system, a total cost of less than €100 kWh−1 and an energy storage size that matches intermittent renewables can greatly strengthen resilience to load fluctuations, grid expansion, and natural disasters. A target of more than (>) 10 kWh m−3 for long-term storage remains with capacity loss < 10% per year (Balasubramaniam et al., 2020).

9.1. Portable and Wearable Electronics

The need for energy storage solutions for portable and wearable electronics is increasing, but it is not fully met. As a result, batteries and supercapacitors have been researched to enable the manufacture of comfortable devices that support movement while offering an ample energy budget. Energy density is the same requirement that we also impose on conventional energy storage devices. This is the amount of available energy per unit weight or area. Materials that work for traditional devices also work for portable and wearable applications, and structures meet the requirements.

According to a study, integrating wearable energy storage devices into clothing and textiles does not hinder comfort, flexibility, or lightness. Furthermore, such energy storage systems enable applications in on-body sensors, artificial skins, and communications and entertainment. Due to the rise of many applications, consumers are now wanting wearable devices. Harvesting energy from body movements, ambient light, and temperature is important for providing self-sufficient energy sources for body-worn electronic devices. Batteries and supercapacitors remain promising candidates for wearable energy storage due to their long cycle life and architecturally compatible form factors. According to Kumar Jha and Subramaniam (2021), supercapacitors, especially hybrid architectures, have unique capabilities such as fast charging and electronic signal modulation that support data transmission and thus are compatible with wearables.

9.2. Electric Mobility and Grid Storage

The push to electrify urban transport and the growing share of renewable energy in the global energy supply chain have created new storage needs. As Li-ion technology has proven successful in portable electronics, the quest for materials for electric vehicles has begun. However, the main target remains long cycle life at an acceptable cost (Czagany et al., 2024). The focus for Li-ion systems has shifted away from energy density to safety, scalability, fast charge and overall cost after a rapid development phase. In the case of stationary storage, the transition from utility-scale storage to grid-scale applications of self-balancing storage technologies, such as flow batteries, has spurred intensified research into the high-throughput selection of redox-active materials (Asghar et al., 2024). As a result, targeted system-level requirements are key parameters for materials selection and device configuration.

9.3. Renewable Energy Integration

The value of grid electricity storage systems varies with fluctuations in supply and demand. Across time scales from seconds to months, load changes occur, while local climate and weather cause renewable generation to be intermittent. Market prices incentivise the storage of energy when supply is abundant, so that when demand increases, energy can be sold on the grid. Energy storage enables the use of low-carbon energy by shifting loads to avoid generating additional fossil-fuel power. Backup supply can be made available for extended periods without causing significant pollution or requiring reliance on out-of-state sources. This can improve grid resilience.

Many devices perform such functions. Energy-intensive Li-based and high-power supercapacitor devices are usually situated in isolated grid zones. Large reservoirs of cooling, firefighting materials, and clean energy have become necessary due to thermal runaway affecting both device types. The banking of supercapacitor devices permits deployment using a corporation's pre-existing electrical infrastructure, and the existing banking of relatively small numbers of low-voltage cells in series within a corporation's facility does not overly engineer the cells. Cleaning and, in many cases, excavation of large mineral resources are required for both Li-based and supercapacitor devices. Another way, with much lower energy density, is to use local batteries for local supply instead of cycling electricity through the grid: eliminating transformers, transmission lines, and other losses reduces overall cooling and cost.

Sodium-ion, zinc, aluminium, and lithium plug)gy systems have lower energy density than what charging them through the grid would allow. These will only compete with lithium-consuming battery-based systems. They have more benefits and disadvantages depending on supply, availability, circulatory turnover, and reversibility. Sustainability depends on the ongoing ability of the geospatial and geophysical computer game, which is Earth, to furnish the necessary materials for the continued construction and usage of these devices.

10. Sustainability, Lifecycle Assessment, and Policy Perspectives

Lifecycle assessment and sustainability are important considerations in evaluating energy technologies (Ager-Wick Ellingsen et al., 2016). The methods of life cycle assessment (LCA), including matrix approaches and 'streamlined' LCAs, help trace environmental impacts in products. Consideration must be given to the following stages: acquisition of raw materials, ancillary materials, manufacture, distribution, use, recycling, and disposal. The principles of green chemistry promote the selection of eco-friendly materials and processes. The efficiency and durability of energy-storage materials can be improved by using nanostructured electrodes and alloy-based anodes. Challenges to the durability of PEM fuel cells, as well as strategies to mitigate degradation, are actively researched. We cannot only consider driving behaviours and the mix used for power generation. Also, we cannot ignore battery weight and the reduction in active materials as development progresses. Standardised tools like ReCiPe and Ecoinvent enable systematic impact assessments. The process of implementing sustainability in energy policy requires a critical assessment of whether adopting technologies offers economic advantages despite significant environmental damage (de Jesús Illera Perozo, 2019).

11. Conclusion

To give this the edge in performance, sustainability, cost, and recyclability, we need materials breakthroughs, be it in Li-ion batteries, hybrid capacitors, or supercapacitors. A lot has been accomplished, but we have much left to do. Future studies can have a significant impact by addressing the root causes of excessive lithium inventory, slow ion and electron transport, interphase instability, electrolyte decomposition, and mismatched chemistries. Energy storage is a key research area, and investment worldwide is growing as a result of climate change, widespread electrification, and clean energy transitions.

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