

# Prospective Competence of Magnesium-ion over Lithium-ion Batteries in Electric Propulsion

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**Abstract.** The rising demand for sustainable electric propulsion led to extensive research on alternative battery chemistries beyond lithium-ion systems. Even though, lithium-ion batteries (LIBs) currently serve as the primary energy storage technology in electric vehicles (EVs), concerns related to resource criticality, dendrite induced safety hazards, and environmental impact prompted interest in magnesium-ion batteries (MIBs). As a potential replacement, MIBs offer several inherent advantages, including the use of Earth abundant and non-toxic magnesium, absence of dendrite formation, high theoretical volumetric capacity, and improved thermal stability. The present review deals with comprehensive comparison of LIBs and MIBs based on electrochemical performance, safety parameters, ion transport characteristics, cycle life, and environmental considerations. Special focus is given to recent developments in MIB component materials, such as bismuth-based and titanium-based anodes, transition metal oxide and chalcogenide cathodes, and hybrid or solid-state electrolytes that support reversible  $Mg^{2+}$  transport. EVs enabled with MIBs can reduce the net CO<sub>2</sub> footprint nearly to 24,800 kg when compared to 26,500 kg and 37,500 kg associated respectively with LIB powered EVs and ICEVs for a span of 10 years. As electrification becoming central to all powertrain architectures, the analysis highlights that although MIBs remain at a lower technology readiness level, their favorable energy densities, extended cycling stability, and reduced ecological footprint position them as strong candidate for future EV battery applications.

**Keywords:** Li-ion batteries, Mg-ion batteries, Electric propulsion, Environmental impact.

## 1 Introduction

Price escalation and adverse environmental impacts of depleting fossil fuels attracted research and implementation towards cleaner alternative powertrains. Among the potential options, electric vehicle can be considered as a promising eco-friendly alternative due to their zero emissions and can extensively reduce greenhouse gas like nitrous oxides (N<sub>2</sub>O), methane (CH<sub>4</sub>), carbon dioxide (CO<sub>2</sub>) etc emissions produced by the transportation sector [1]. Electric vehicles (EVs) offer energy conversion efficiencies of 80–95% even at high torque even at low speeds. They also provide rapid and precise torque output, often exceed

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the rated power by 2–3 times. Rechargeable batteries are vital components that has ascertain influence on the performance as well as environmental impact of electric vehicles. Lithium-ion batteries (LIBs) are the most commercially viable energy storage option among the batteries used in electric propulsion. LIBs commonly use cathodes like  $\text{LiCoO}_2$  and  $\text{LiFePO}_4$ , paired with graphite or high-capacity anodes like Si or Sn composites, supported by organic or polymer-based electrolytes and polyolefin separators that ensure safe ion transport [2]. Present range limitation of electric vehicles can be mitigated in future by replacing LIBs with higher charge density magnesium-ion batteries (MIBs). MIBs typically use metallic magnesium or alloy-based anodes, sulphur or Chevrel phase cathodes for high energy density, and liquid or solid electrolytes like Grignard or boron-based types to ensure reversible ion transport and stability [3]. As per the technological landscape, LIBs are currently chosen for their high energy density, mature technology, and proven performance in EVs while, MIBs are to be explored for their superior safety, lower cost, and environmental sustainability. Together, LIBs and MIBs respectively represent the present and future solutions for efficient and greener electric mobility. A broad spectrum of recent literature addresses critical aspects of LIB technology pertaining to materials selection, modelling, diagnostics and recycling. Martí-Flores et al. [4] reviewed the gap between theoretical designs of LIBs and their industrial implementation, thereby serving as a practical guide for the development of new LIB applications. Kabir and Demirocak [5] delved into electrolyte related degradation mechanisms and identifying the growth of the solid electrolyte interphase (SEI) as a primary contributor to capacity deterioration and internal resistance in LIBs. Deng [2] provided a foundational overview of LIBs and highlighted the challenge posed by low volumetric density of nanomaterials, proposing micromaterials composed of nanoparticles to enhance material compaction. In diagnostics, Raccichini et al. [6] reviewed the use of reference electrodes (REs) and advocated for materials such as partially de-lithiated  $\text{LiFePO}_4$  that offers superior potential stability compared to lithium metal. Further, Kim et al. [7] focused on next-generation battery materials and emphasized the urgent need for safe recycling practice and highlighted the risk of fire from undischarged cells during recycling processes. Building on the limitations and challenges associated with LIBs, recent research focused towards MIBs as promising alternatives, particularly due to their material abundance, safety, and multivalent charge capabilities. Zhan et al. [8] reviewed recent advances in Mg-ion solid conductors and noted a significant improvement in ionic conductivity from  $10^{-3} \text{ S cm}^{-1}$  at  $800^\circ\text{C}$  to  $10^{-4} \text{ S cm}^{-1}$  at room temperature through the application of materials such as phosphates, borohydrides, chalcogenides, and metal-organic frameworks (MOFs). Massé et al. [9] highlighted the higher theoretical volumetric capacity ( $3832 \text{ mAh cm}^{-3}$ ) and inherent advantage of non-dendritic deposition of Mg-ion electrode material compared to Na-ion electrode material. They also emphasized the exceptional cycling stability of chevrel phases as the cathode material. Kiai et al. [10], [11] broadened the scope to various multivalent metal-ion batteries and identified Mg-ion batteries as highly suitable for electric vehicles due to their safety, sustainability, energy storage potential, low cost, and environmental benefits. Ma et al. [11] further explored cathode materials and electrolyte compatibility by recognizing Chevrel phase  $\text{Mo}_6\text{S}_8$  as the first cathode that supports reversible cycling with multiple Mg electrolytes, delivering over  $50 \text{ mAh g}^{-1}$  for 500 cycles. They also highlighted magnesium organoborate electrolytes for their ability to enable reversible magnesium plating. Moreover, magnesium provides an opportunity for cycling two electrons compared to single electron cycling that in lithium-ion systems [12]. Also, LIB tends to face thermal runaway, where puncture or mechanical damage can trigger rapid heat release and cell destabilization. In contrast, MIB technology with improved intrinsic safety, is still widely viewed as being in an early developmental stage and requires further refinement in terms of materials optimization and electrochemical performance to attain commercial maturity [13]. From the

detailed review, no manuscript is found to be reported on the comprehensive comparison of electrochemical, environmental, safety, and techno-economic attributes of lithium-ion and magnesium-ion batteries. This paper deals with the detailed comparison of the performance, sustainability, and future readiness of LIBs and MIBs for electric propulsion.

## 2 Description of Li-ion and Mg-ion batteries

### 2.1 Li-ion Battery

Lithium-ion battery (LIB) generates electrical energy through electrochemical redox reactions in the cathode and anode supported by the exchange of lithium ions. The rechargeable system is generally comprised of anode, cathode, electrolyte and a microporous solid polymer membrane separator. Cathode is typically a lithium metal oxide such as lithium cobalt oxide ( $\text{LiCoO}_2$ ), lithium iron phosphate ( $\text{LiFePO}_4$ ), lithium nickel cobalt aluminium oxide ( $\text{LiNi}_x\text{Co}_y\text{Al}_z\text{O}_2$ ), lithium titanate oxide ( $\text{Li}_4\text{Ti}_5\text{O}_{12}$ ), lithium nickel manganese cobalt oxide ( $\text{LiNi}_x\text{Mn}_y\text{Co}_{1-x-y}\text{O}_2$ ) [7]. The solid membrane is permeable for  $\text{Li}^+$  to ensure its reaction with cathode in the discharging mode but blocks and force the electrons to flow through the external circuit to contribute the required current. The relative flow of ions and electrons in LIBs during charging and discharging is respectively depicted through Fig. 1(a) and (b). Even through alloys materials, transition metal oxides and silicon-based compounds can serve as anode, carbon-based anodes like graphite are commercially preferred due to its ample availability, low cost, excellent electronic conductivity, flat potential profile during charging and discharging along with favourable structure for ion intercalation to facilitate efficient charging and discharging cycle [14]. The electrolyte in LIBs typically comprises a lithium salt like  $\text{LiPF}_6$  in organic carbonate solvents, enabling  $\text{Li}^+$  transport and SEI formation. During the discharging cycle, the anode undergoes oxidation, and the released electrons and ions are respectively driven to the cathode via the membrane and external circuit to facilitate reduction reaction. The anode, cathode and overall reactions of LIB with lithium cobaltate as cathode and lithiated graphite as anode is given in equations (1), (2) and (3).

Anode reaction



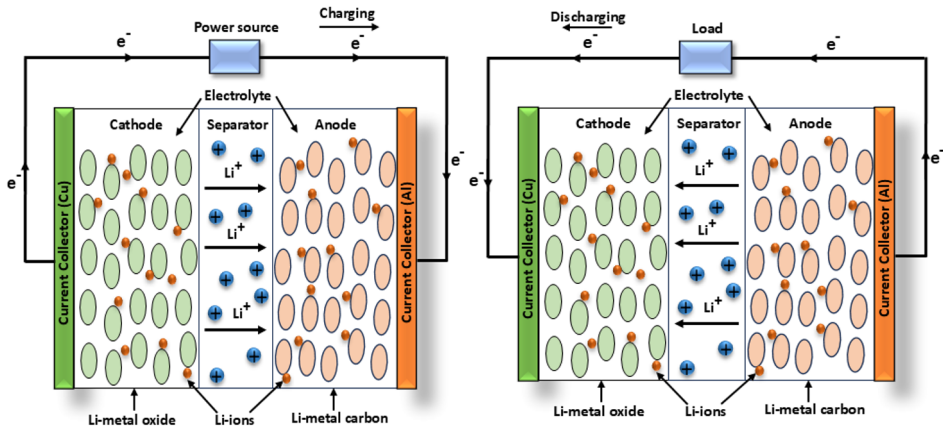
Cathode reaction



Overall reaction



Attributes such as prolonged service, fast charging, better single cell voltage, high specific energy and efficiency designated LIB a pioneer among the batteries employed for electric propulsion [15].



**Fig. 1.** Schematic of Lithium-ion battery (a) charging (b) discharging

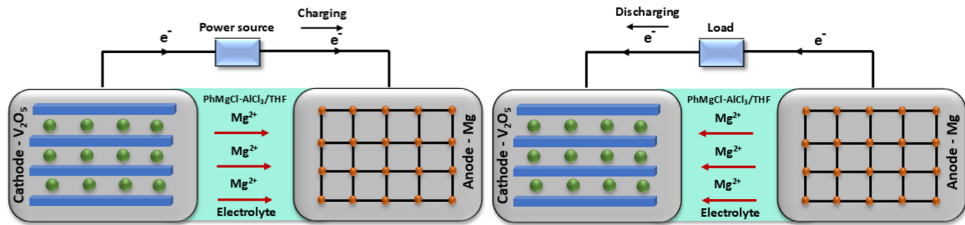
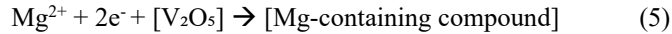
## 2.2 Mg-ion Battery

A typical magnesium-ion battery (MIB) system consists of a cathode, anode, electrolyte, and current collectors, with overall performance critically dependent on the interfacial and structural properties of these components. Aurbach et al. developed the first MIB prototype using a Chevrel phase cathode ( $\text{Mo}_6\text{S}_8$ ), a magnesium metal (Mg) anode, and an organohaloaluminate-based electrolyte. Cathode materials should offer high operating voltage, good magnesium-ion reversibility, high energy density, and low cost. Selecting suitable cathode materials is challenging due to the strong polarization of  $\text{Mg}^{2+}$  ions, which hampers reversible capacity and power output. Common cathode materials for MIB include Transition Metal Chalcogenides (TMCs) such as Chevrel phases ( $\text{M}_x\text{Mo}_6\text{X}_8$ ) and  $\text{MS}_2$  ( $\text{M} = \text{Ti}, \text{Mo}$ ), transition metal oxides such as  $\text{V}_2\text{O}_5$ ,  $\text{MnO}_2$ ,  $\text{MoO}_3$  and polyanion compound such as phosphates, silicates. Frequently used electrolytes include  $\text{Mg}(\text{ClO}_4)_2$ ,  $\text{Mg}(\text{PF}_6)_2$ , and  $\text{Mg}(\text{TFSI})_2$  in carbonate or ether solvents. A key limitation is the irreversible formation of passivation layers on the Mg anode. The all-phenyl complex (APC) electrolyte supports reversible Mg plating or stripping but suffers from low voltage, corrosiveness, and impracticality. Anodes in magnesium-ion batteries (MIBs) must deliver high specific and volumetric capacities, low operating voltage, chemical stability with electrolyte, and must also be cost-effective, environmentally benign, and electrically conductive [3]. A standard MIB setup typically uses magnesium (Mg) as the anode, vanadium pentoxide ( $\text{V}_2\text{O}_5$ ) as the cathode, and a  $\text{PhMgCl}-\text{AlCl}_3/\text{THF}$  solution as the electrolyte. During discharge, magnesium oxidizes at the anode, releasing  $\text{Mg}^{2+}$  ions that migrate through the electrolyte and intercalate into the cathode. Electrons simultaneously flow through the external circuit, producing electrical energy. During charging, the process reverses under an applied voltage, restoring the battery's original state. Magnesium is oxidized in the anode, releasing  $\text{Mg}^{2+}$  ions and electrons as seen in equation (4) whereas in cathode, magnesium ions are inserted into the cathode material, and electrons are consumed as in equation (5) forming, Mg-containing compound. The electrolyte facilitates the movement of  $\text{Mg}^{2+}$  ions between the electrodes. Common electrolytes include magnesium salts dissolved in organic solvents.

Anode (Magnesium metal):



Cathode (Metal oxide or other material):



**Fig. 2.** Schematic of Magnesium-ion battery (a) charging (b) discharging

### 3 Comparison of Lithium-ion and Magnesium-ion batteries

**Table 1.** Comparison of different parameters of Li-ion and Mg-ion battery.

Parameters	Li-ion Battery	Mg-ion Battery
Ion-Diffusion Coefficient	$10^{-10} - 10^{-9} \text{ cm}^2 \text{ s}^{-1}$ ( <b>T</b> : 298 K, <b>E</b> : Graphite anode and layered metal oxide cathode, <b>ELEC</b> : commercial organic electrolyte LP50 (BASF))	$1.1 \times 10^{-9} \text{ cm}^2 \text{ s}^{-1}$ ( <b>T</b> : 300 K, <b>E</b> : Magnesium metal anode and Magnesium Iron Silicate cathode, <b>ELEC</b> : Mg-ion based electrolyte)
Dendrite Formation	High	Absent
Gravimetric energy density ( $\text{Wh kg}^{-1}$ )	$<250 \text{ Wh kg}^{-1}$ ( <b>E</b> : Graphite anode and Lithium-cobalt oxide cathode, <b>ELEC</b> : liquid-salt containing lithium)	$874 \text{ Wh kg}^{-1}$ ( <b>E</b> : Magnesium metal anode and Sulphur-cathode, <b>ELEC</b> : (HMDS) <sub>2</sub> Mg- based electrolyte)
Volumetric energy density ( $\text{Wh L}^{-1}$ )	$<650 \text{ Wh L}^{-1}$ ( <b>E</b> : Graphite anode and Lithium-cobalt oxide cathode, <b>ELEC</b> : liquid-salt containing lithium)	$3200 \text{ Wh L}^{-1}$ ( <b>E</b> : Magnesium metal anode and Sulphur cathode, <b>ELEC</b> : (HMDS) <sub>2</sub> Mg- based electrolyte)
Power Density ( $\text{W/kg}$ )	$340 \text{ W kg}^{-1}$ ( <b>E</b> : Graphite anode and Lithium-cobalt oxide cathode, <b>ELEC</b> : liquid-organic containing lithium)	$1440 \text{ W kg}^{-1}$ ( <b>E</b> : Lithium Vanadium Phosphate anode and Poly-pyrometallitic dianhydride cathode, <b>ELEC</b> : aq

		aqueous magnesium ion electrolyte)
Activation Energy (eV)	Li <sub>7</sub> Ti <sub>5</sub> O <sub>12</sub> : 0.20–0.51 eV Li <sub>2</sub> CO <sub>3</sub> : 0.7 eV	MgTiO <sub>3</sub> : 0.88 eV Mg <sub>3</sub> Fe <sub>2</sub> Si <sub>3</sub> O <sub>12</sub> : 2.19 eV
Charge-Rate in terms of C	0.2C, 0.5C, 1C, and 1.5C ( <b>T</b> : 298 K, A18650 commercial model type of Li-ion battery)	0.1 C, 0.2 C, 0.5 C, 1 C, and 2C ( <b>T</b> : 298 K, <b>E</b> : Magnesium metal anode and Mo6S8 Chevrel phase cathode, <b>ELEC</b> : Mg-based electrolyte)
Discharge-Rate in terms of C	0.5C, 0.9C, 1.3C, and 1.6C ( <b>T</b> : 298 K, A18650 commercial model type of Li-ion battery)	0.1 C, 0.2 C, 0.5 C, 1 C, and 2C ( <b>T</b> : 298 K, <b>E</b> : Magnesium metal anode and Mo6S8 Chevrel phase cathode, <b>ELEC</b> : Mg-based electrolyte)
Battery Cycles	(LCO) : 500–1000 cycles (NMC) : 1,000 cycles (NCA) : 2000 cycles (LFP) : >2000 cycles	(AMIB): 1000 cycles at 2 C and for 6000 cycles at 20 C.
Thermal Capacity	0.90 - 0.975 J g <sup>-1</sup> K <sup>-1</sup> (NCA) 0.83-1.0118 J g <sup>-1</sup> K <sup>-1</sup> (LiCoO <sub>2</sub> )	-----
Technology Readiness Level (TRL)	High TRL-9	Low TRL 1-3

A detailed comparison of LIBs with MIBs is presented in table 1. The ion-diffusion coefficient, which influences ion transport speed within the cell, is slightly higher in MIBs ( $1.1 \times 10^{-9} \text{ cm}^2 \text{ s}^{-1}$ ) compared to LIBs ( $10^{-10} - 10^{-9} \text{ cm}^2 \text{ s}^{-1}$ ), though both are within the same magnitude. Dendrite formation, a critical safety concern, is prominent in LIBs but absent in MIBs, making the latter intrinsically safer. With respect to gravimetric energy density (energy per unit mass), MIBs show superior performance ranging from 180 Wh/kg to 874 Wh/kg depending on the cathode material compared to a value < 250 Wh/kg for LIBs. Recent studies indicate that Mg-ion batteries can meet practical energy density requirements, positioning them as a promising alternative with performance levels comparable to advanced Li-ion systems. Similarly, volumetric energy density (energy per unit volume) is significantly higher for MIBs (3200 Wh/L) than LIBs (<650 Wh/L). These two parameters directly influence the battery's size and weight, higher gravimetric energy density enables lighter batteries for the same energy output, while higher volumetric energy density allows for more

compact battery packs. Power density, which indicates how rapidly energy can be delivered, is also notably higher in MIBs (1440 W/kg) compared to LIBs (340 W/kg), contributing to better performance and potential reduction in total system weight due to fewer parallel cells needed for high-power applications. Regarding activation energy, MIBs require more energy (0.52–2.19 eV) for  $Mg^{2+}$  migration compared to  $Li^+$  in LIBs (0.2–0.7 eV), which increases resistance to ion movement and limits overall charge–discharge efficiency, especially at high rates. The charge and discharge rates, expressed in C-rates, are comparable across both the systems. LIBs typically operate between 0.2C to 1.5C for charging and 0.5C to 1.6C for discharging, while MIBs support 0.1C to 2C for both the processes, offering flexibility in cycling behaviour under optimized conditions. The cycle life, which measures the number of charge–discharge cycles before significant capacity downfall, generally favours MIBs. Under controlled conditions some MIBs configurations demonstrate up to 6000 cycles whereas LIBs typically range between 500 to 2000 cycles depending on battery configuration. This suggests MIBs could offer longer operational lifespans with reduced replacement needs. Thermal capacity, a measure of the battery’s ability to absorb heat, is documented for LIBs (0.83 to 1.01 J/g·K), aiding in thermal management during rapid cycling or external temperature variations. However, equivalent data for MIBs under research, making it difficult to assess their thermal safety performance under similar stress conditions. Finally, from a technological standpoint, LIBs are commercially mature with a Technology Readiness Level (TRL) of 9, supported by established industrial infrastructure and supply chains. In contrast, MIBs remain at an early development stage (TRL 1–3), requiring further advancements in material design, electrochemical analysis, and full-system implementation. Performance metrics of MIBs offer notable economic and environmental advantages over LIBs. Magnesium is eight times more abundant than lithium and costs roughly one-third as much, providing a strong pathway for long-term material cost reduction, while its high volumetric capacity enables more compact and lower-cost battery packs. Even though, current development is constrained by the expensive and complex synthesis of advanced electrolytes such as carborane and aluminate salts, the overall material cost outlook remains favourable. From the sustainability perspective, MIB manufacturing is less energy-intensive and generates fewer toxic by-products. Moreover, the absence of dendrite formation supports a longer cycle life, thereby enhancing life-cycle energy gain. While mature recycling pathways for MIBs are not yet established, magnesium’s inherently non-toxic, stable chemistry indicates potential for simpler and safer end-of-life processing compared to the energy-intensive and environmentally burdensome recycling of LIBs.

## 4 Environmental Impact

The rapid increase of electric vehicles (EVs) is widely regarded as a significant step towards a sustainable future development by effectively mitigating air pollution and greenhouse gas (GHG) emissions. In this transition, LIBs have emerged as the dominant technology in EV applications and are seen as crucial elements for a future low-carbon economy, enabling the widespread adoption of renewable energy sources and the decarbonization of the transport sector. However, the positive environmental aspects of EVs can be completely ensured if and only if the material employed for battery design do not pose any environmental threats. The production of certain LIB components particularly nickel and cobalt used in cathodes is recognized as a major contributor to environmental impacts, especially in terms of Human Toxicity Potential (HTP). Among LIBs, Lithium Iron Phosphate (LFP) batteries generally demonstrate reduced environmental impact due to the absence of these metals which irradiates the toxicity and usage of resource-intensive materials. LFP-LTO battery systems exhibit notably favourable lifetime environmental impacts, primarily due to their

exceptionally high cycle life compared to other established battery chemistries. While LFP chemistries typically have lower specific energy and may present higher greenhouse gas (GHG) emissions per watt-hour of storage capacity, their extended operational lifespan enables the environmental costs associated with production to be distributed over a far greater number of charge-discharge cycles. As a result, when evaluating batteries based on total lifecycle performance rather than per-cycle metrics, LFP-LTO configurations emerge as among the most promising options in terms of long-term sustainability and resource efficiency. Remanufacturing LIBs by using recycled materials from used batteries can significantly reduce GHG emissions, water consumption, and production costs compared to manufacturing with virgin materials [39]. Compared to Pyrometallurgical Recycling (PR) and Hydrometallurgical Recycling (HR), Direct Physical Recycling (DPR) demonstrates the highest potential for reducing greenhouse gas (GHG) emissions (29.27%–38.15%), water consumption (30.07%–41.19%), and overall costs (25.61%–36.63%) even at its infant stage. In terms of battery chemistries, remanufacturing NCM111 cells via DPR yields the lowest environmental impact across key categories. Additionally, NCA batteries exhibit notable GHG emission reductions during manufacturing compared to NCM variants, despite the relatively early stage of NCA technology development. In fact, overall recycling not only contributes significantly to reduce emissions by replacing the need for virgin materials but also avoids the environmental burden associated with ore extraction and refinement. Safer disposal practices and the use of less hazardous battery chemistries offer clear environmental and safety advantages. Landfilling or incinerating LIBs leads to severe environmental contamination and health risks due to the release of heavy metals, HF, and toxic gases. Moreover, frequent fires and explosions in waste streams further elevating the hazards. Considering the disposal and lifecycle of LIBs, current research efforts are increasingly directed towards the development of alternative battery chemistries with enhanced sustainability and reduced ecological impact. MIBs present several compelling advantages over LIBs through its abundant availability of magnesium and its non-toxic and safe nature for handling in ambient air compared to lithium and absence of dendrite formation in MIBs reduces fire explosion and risk. Prospective Life Cycle Assessment (LCA) for vehicles over a 10-year lifetime covering 150,000 km, assuming an EV battery capacity of 40 kWh [3]. Environmental Impact in the revised manuscript Life Cycle Assessment (LCA) studies indicate that the cumulative cradle-to-use CO<sub>2</sub>-equivalent emissions for MIBs employing sulphur-based electrode in electric vehicle (EV) are approximately 24,800 kg which is marginally lower than that of a lithium-ion battery (LIB) EV (~26,500 kg) and substantially lower than a conventional internal combustion engine vehicle (ICEV), which emits around 37,500 kg over a decade. This is partly due to the lesser CO<sub>2</sub>-intensive construction of the Mg-ion battery pack. Moreover, this MIB in EVs has demonstrated superior performance in terms of acidification potential, contributing only about 75–77% of the impact associated with LIB EVs and ICEVs, this is attributed to the less critical supply chain of electrode active materials for Mg-ion batteries, avoiding significant emissions of acidifying agents seen in nickel sulphate production for Li-ion batteries. Currently, MIBs are gaining continual research attention as a viable next-generation energy storage solution for EV applications due to their potential advantages in material abundance, safety, and environmental compatibility.

## 5 Future research direction

LIBs currently hold the top position among rechargeable power sources for consumer electronics and remain key candidate for EV propulsion systems. They have undergone significant advancements over the last decade, becoming a mature and reliable technology with still considerable improvement potential. MIB technology faces key material

challenges, mainly the slow movement of  $Mg^{2+}$  ions and the lack of electrolytes that work well with common electrode materials. These issues often lead to the formation of an electrically insulating passivation layer on Mg that blocks transfer of  $Mg^{2+}$  ions in smooth plate and strip processes. In contrast, the solid electrolyte interphase (SEI) on Li metal is naturally conductive  $Li^+$  that allows continuous ion flow and ensures more stable electrochemical cycles in LIB systems. Despite wide deployment and clear benefits, LIBs face technical hurdles, and their limited theoretical energy and specific energy capacities restrict the EV performance. Moreover, reduction on the battery lifespan also leads to power loss, limited output, and other safety concerns. Researchers seek ways to improve LIB performance through material upgrades that provide better safety, extended life, and faster charge time. In this context, lithium-sulphur (Li-S) and lithium-oxygen (Li-O<sub>2</sub>) variants show strong potential for higher energy yield and charge capacity, even though adversely affected by, such as electrolyte loss, dendrite growth, and inorganic layer buildup at electrodes. Research associated with incorporation of solid-state battery (SSB) frameworks into LIB systems are in progress to tackle these issues. In this view, innovative materials such as  $LiTi_2(PS_4)_3$  (LTPS) are introduced to increase lithium-ion diffusion within solids for enhanced conductivity and safety. However, proper and timely recycling methods remain vital for LIBs to reduce environmental impact as well as cost by cutting down the raw material demand. Currently, Artificial Intelligence (AI) and Machine Learning (ML) support prediction of material traits and reduce development cycles. These tools also help to build smarter Battery Management Systems (BMS), which improve fault checks, output control, and system safety. MIBs now gain interest as next-generation alternatives to LIBs, especially for grid-scale storage due to magnesium's high abundance (about 2.3% of Earth's crust) and lower cost. Apart from cost, MIBs also offers better safety during production and operation stages. Recycling approaches differ due to material properties and lifecycle impacts. MIB manufacturing is less energy-intensive and environmentally safer, as magnesium forms no toxic compounds, unlike Li-ion batteries, whose disposal demands high energy and poses greater environmental risks. Lower reactivity of magnesium in air makes its handling safer compared to lithium or sodium during battery production. MIBs also offers better safety under repeated charge and discharge cycles due to the absence of dendrite growth. Moreover, magnesium proves ideal for compact energy systems as it ensures a theoretical volumetric capacity nearly twice that of lithium. Also, magnesium compounds show low or no toxicity, which supports their eco-friendly profile. Despite of all these positive aspects, MIBs demand further research as it faces key scientific and commercial obstacles. Magnesium ions ( $Mg^{2+}$ ) have poor mobility and limited solid-phase transport, due to their dual charge and high polarization, which reduces output and limits reversibility. Most lithium-compatible cathodes reject  $Mg^{2+}$ , as divalent ions face strong electrostatic pushback from host electrodes. On the cathode sides, studies aim to address low energy storage and weak kinetics by adjusting oxide structures to ease  $Mg^{2+}$  movement and reduce ion-host friction. Development of durable cathodes with improved energy yield in 2–3 V range are under research to overcome these bottlenecks. Improvisation of material challenges in MIBs include removal of non-reversible passivation layers from magnesium surfaces, adoption of artificial solid electrolyte interfaces (SEIs), use of nano-scale Mg forms, and design of Mg-based alloy anodes with elements like bismuth or tin along with structural strain concerns. Materials such as  $Li_4Ti_5O_{12}$ , along with two-dimensional forms like defective graphene, phosphorene, and arsenene, show promise as Mg-ion hosts. Micro-alloy types, for example Mg-Ca-In, have shown gains in anode voltage and efficiency with less corrosion [46]. Electrolyte working also plays a vital role in the performance of MIBs, directly influencing  $Mg^{2+}$  transport, stability, and reversibility. Focus now shifts to affordable and stable liquid types with chelating agents like methoxyethyl amines, which enhance  $Mg^{2+}$  extraction, lower overpotentials, and boost transport. In aqueous setups, complex agents prevent iron accumulation and suppress the formation of

Mg(OH)<sub>2</sub> residue, thereby increased charge yield. Solid-state electrolytes represent an alternative approach in MIBs development, with perovskites, anti-perovskites, phosphates, chalcogenides, borohydrides, and MOF-based solids offering better Mg-ion flow. Ongoing research aims to transfer photo-charging design principles to MIB chemistries, although multivalent Mg<sup>2+</sup> ions diffusion kinetics and electrolyte–electrode interfacial compatibility remains critical barriers in achieving comparable system efficiencies. Finally, AI and ML models support prediction of performance, corrosion as well as electrochemical trends and also optimize material choice to speed up MIB design for EVs and large-scale grid power systems.

## 6 Conclusions

A comprehensive review was conducted to provide a detailed comparison on the electrochemical, environmental, safety, and techno-economic attributes of LIBs and MIBs for electric propulsion applications. A broad range of recent literature covering the key aspects such as material selection, model development, diagnostics, and recycling methods are reviewed for both LIBs and MIBs technology. Despite technological maturity and market leadership, LIBs face critical technical and environmental challenges. This includes safety risks posed by dendrite growth, fire hazards from residual charge in discarded cells, as well as adverse environmental impacts pertaining from disposal and incineration along with the extraction and processing of metals for LIB cathodes. Among LIB variants, Lithium Iron Phosphate (LFP) cells stand out for their absence of toxic metals and long service life. Improvement strategies for LIBs currently include the adoption of lithium-Sulphur and lithium-oxygen chemistries, along with a shift to solid-state battery architectures. On other hand, MIBs are emerging alternative in terms of safety, cost, and environmental aspects even in the early stage of development. They appear intrinsically safer due to the absence of dendrite formation and also demonstrate better energy and power performance, along with extended cycle life. EVs enabled with MIBs can reduce the net CO<sub>2</sub> footprint nearly to 24,800 kg when compared to 26,500 kg and 37,500 kg associated respectively with LIB powered EVs and ICEVs for a span of 10 years. Apart from the benefits, MIBs face key challenges like low magnesium-ion mobility, poor solid-state transport, magnesium-ion incompatibility with LIB electrodes and higher activation energy required for magnesium migration. Current research focuses on identifying suitable electrode materials, better recycling strategies and stable as well as low-cost electrolytes. The commercialization in rechargeable magnesium batteries (RMBs) hinges on addressing challenges in electrolyte synthesis, cost and interface stability. Magnesium's abundance offers a cost advantage over lithium, and it is compatible with electrolytes such as carborane salts suffer from complex, moisture-sensitive and expensive synthesis routes. Current research on MIBs focuses on additive engineering to improve anode–electrolyte interfaces, developing solid or quasi-solid polymer electrolytes (e.g., Mg[B(hfip)<sub>4</sub>]<sub>2</sub>) for enhanced stability and safety, and creating simpler as well as scalable synthesis pathways to enable practical full-cell RMB deployment. Researchers use Artificial Intelligence (AI) and Machine Learning (ML) tools to predict battery performance, material properties, electrochemical compatibility, corrosion behavior along with design and optimization Battery Management Systems (BMS). Even though under early development stage, concentrated research efforts and the application of advanced digital tools can enable the transition towards magnesium-based systems. This shift holds the potential to redefine electric propulsion with safer, cost-effective, and environmentally sustainable battery solutions.

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