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Sustainable cathode material screening for sodium-ion batteries using a hesitant fuzzy-intuitionistic MCDM framework

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Sodium-ion batteries (SIBs) present a promising alternative to conventional lithium-ion batteries (LIBs), offering potential advantages in cost reduction and environmental sustainability. SIBs are in the early stages of development and numerous cathode materials are still being explored. A systematic screening is required to identify the most promising sustainable cathode materials of these early-stage technologies, in line with EU battery regulations and chemical safety strategies. To support such a screening, the evaluation considers major factors such as energy density, cost, greenhouse gas (GHG) emissions, supply risk, and input-related toxicity. As the number of evaluation criteria is high, both the complexity of finding an optimal solution and the impact of linguistic uncertainties in decision-making grow significantly. To address these challenges, a combination of hesitant-intuitionistic fuzzy multi-criteria decision-making (MCDM) is proposed. The hesitant fuzzy linguistic Analytic Hierarchy Process (HFL-AHP) is used to assign weights to the criteria, while the intuitionistic New Easy Approach to Fuzzy-PROMETHEE (NEAT-Fuzzy-PROMETHEE) method is used to rank the alternative materials. Obstacle degree analysis and comprehensive sensitivity assessments are additionally performed to find the field of improvement and ensure robustness with reliability of the results, respectively. The results highlight that the energy density of the cathode material is a critical factor in the screening of optimal solutions. Na_2FeSiO_4 is the optimal solution when input-related toxicity is not included, while $Na_{0.61}Fe[Fe(CN)_6]_{0.94}$ † becomes a promising option with the inclusion of that factor under given assumptions and limitations of the approach. Furthermore, the analysis shows that energy density, GHG emissions and toxicity affect sustainable decision-making in material screening, indicating critical areas for improvement.

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1. The research advances green chemistry through a hesitant-intuitionistic fuzzy decision-making approach that integrates not only technical performance but also environmental, economic, criticality and toxicity indicators. This comprehensive approach identifies low-impact, non-toxic and resource-abundant cathode materials – Na_2FeSiO_4 and $Na_{0.61}Fe[Fe(CN)_6]_{0.94}$ – as an optimal solution for greener sodium-ion battery development, aligning with EU "Safe and Sustainable by Design" principles.
2. This study evaluates a data-driven comprehensive sustainability screening of 23 cathode active materials for sodium-ion batteries through a multi-criteria decision-making analysis. Quantitatively, Na_2FeSiO_4 and $Na_{0.61}Fe[Fe(CN)_6]_{0.94}$ outperformed other cathodes with 60–70% lower toxicity and GHG emissions than NMC cathodes. Qualitatively, this work advances hazard-aware material selection by explicitly integrating environmental safety and regulatory factors into decision-making for sustainable material selection.
3. Future work can enhance greenness by integrating computational sustainability screening with system-level life-cycle data, comprehensive validation, different synthesis processes, recycling efficiency and real-scale manufacturing parameters.

1. Introduction

Batteries are regarded as a potential option to address the challenges associated with the intermittency of renewable energy resources, enabling a flexible, safe and economically viable transition toward a more sustainable energy system.[1] This drives significant market growth in battery technologies, with global battery demand projected to reach 2600 GWh in 2030.[2] To meet this growing demand in a more sustainable

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† Prussian blue analogues.

manner, recent research has focused on post-lithium batteries.[3] These post-lithium (Li) systems include a wide range of cell chemistries, such as sodium (Na), magnesium (Mg), aluminium (Al), calcium (Ca), potassium (K), and zinc (Zn). In this context, SIBs are regarded as one of the most promising alternatives to mitigate the use of critical, toxic and expensive materials with high environmental impact.[4] SIBs share many similarities with LIBs and are often considered a drop-in technology, offering a broad range of potential cathode material options. A key advantage of SIBs is the substitution of Na for Li in both the active materials and electrolytes.[5] It reduces reliance on scarce resources while maintaining comparable electrochemical performance. Additionally, they utilise aluminium as the current collector instead of copper and hard carbon instead of graphite as an anode.[6] Due to the larger ionic radius of sodium, SIB technologies specifically exhibit lower energy density compared to LIBs.[7] Nevertheless, they remain compatible with several application fields, making them a viable alternative in targeted energy storage applications. As a result, SIBs are expected to experience substantial market growth, with a projection to increase from USD 172.8 million in 2022 to USD 270.1 million by 2025, representing a remarkable growth of 56.1%.[8,9] There are several companies and start-ups actively commercialising SIBs across various industries worldwide. According to FutureBatteryLab's 2024 report, the landscape is dominated by a few countries in Europe, America and Asia, who are driving innovations in stationary storage, e-mobility and other applications.[10]

For both SIBs and LIBs, intercalation reactions are required for cathode active materials (CAMs) which allow reversible insertion of a high amount of the guest species like Na^+ and Li^+.[11] Depending on the application, the most useful CAMs for present LIBs are lithium nickel manganese cobalt (NMC) 622 ($LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$), and lithium iron phosphate ($LiFePO_4$ (LFP)).[12] For SIBs, which are at lower technology readiness levels (TRLs), a wide range of material combinations are being explored, each offering diverse properties in terms of energy density, cycle life, coulombic efficiency, cost, resource availability/criticality and environmental impact.[13] These materials are generally classified into two primary categories: polyanionic materials and layered oxides. Additionally, some literature introduces a third classification, Prussian blue analogues (PBAs). Extensive research has analysed the structure and properties of these types of CAMs in detail.[7]

The cathode is a key component that significantly influences the economic and environmental performance of a cell.[14] Therefore, to assess the potential impact of cathodes on economic and environmental factors, it is crucial to evaluate a broad range of material combinations.[15] To minimise sustainability impacts, it is critical to consider the entire lifecycle of these materials, including raw material extraction, purification, manufacturing, transportation, use and end-of-life management.[16] This includes adhering to restrictions on hazardous substances in metal-ion batteries to reduce risks to human health and the environment. Consequently, evaluating hazardous substances is important to address aspects of "safe and sustainable by design (SSbD)" for the metal-ion batteries.[11,17] Therefore, there is a need to develop a methodology that includes several key parameters which can be classified under different sustainability dimensions. This study includes major factors like energy density, cost, greenhouse gas (GHG) emissions, supply risk (SR), end of life recycling input rate (EOL-RIR), import reliability and toxicity, which are categorised under economic, environmental, social, technical and hazards aspects.[18] Different sustainability dimensions lead to complexity and uncertainty in decision-making, leading to different solutions. Therefore, it is essential to add a robust decision-making approach that is able to tackle this complexity with linguistic uncertainty to obtain reliable results.

Most previous studies have assessed technical performance, with few addressing the economic, environmental and criticality aspects of different SIB CAMs.[19–21] There is limited research on screening for the toxicity and hazardous aspects of CAMs.[12] Integrated approaches that simultaneously consider relevant performance factors, such as economic, environmental, technical, safety and criticality, are still lacking for comprehensive CAM screening. This methodological gap, coupled with the inherent complexity of evaluating diverse and interdependent criteria makes the selection process complex. It poses significant challenges for decision-makers aiming to identify the most sustainable CAM option. Additionally, the uncertainty arising from the qualitative nature of many criteria and subjective judgement remains insufficiently addressed in current material screening methodologies. This creates more difficulties for decision-makers to identify the most suitable solution. Furthermore, decision-makers must understand the key factors that influence CAM selection for further development and identify the performance enhancements needed to ensure competitiveness.

1.1. Research objectives and contribution

Considering the identified research gaps, this study proposes a hierarchical and comprehensive methodology to screen various CAMs of SIBs and ranks the alternatives based on key factors categorised under sustainability dimensions. The screening process includes techno-economic factors such as energy density, CAM cost, EOL-RIR and economic importance. Additionally, GHG emissions of different CAMs are evaluated to quantify the carbon footprint of each technology, thereby providing insights into their environmental impacts.

Furthermore, the methodology integrates critical supply-related factors, including SR and import reliability, to ensure a holistic sustainability assessment. Beyond the current state-of-the-art, this study also introduces hazard and toxicity screening assessment as an additional evaluation criterion for identifying an optimal CAM option. For this purpose, revised and up-to-date data for each CAM across the selected sustainability dimensions are utilized based on previously discussed sources.[5,12]

Since the considered CAMs are at varying stages of technological maturity (early-stage to market ready), the identification of an optimal alternative includes uncertainty in decision-making. Moreover, the inclusion of multiple evaluation criteria further increases the complexity of the decision-making process. To address these challenges, namely complexity, hesitancy and uncertainty in decision-making, this study adopts a robust hesitant intuitionistic MCDM methodology. The HFL-AHP and the NEAT-Fuzzy-PROMETHEE methods are applied to determine the weights of the criteria and rank the alternatives within this uncertain environment, respectively.

Additionally, a novel obstacle degree model is proposed to identify and quantify barriers imposed by specific criteria that may obstruct the identification of optimal CAMs. This also helps to identify the potential hotspots of future improvement of the considered CAMs. To ensure the prospectiveness and reliability of the results, extensive sensitivity analyses are conducted, along with the future scenario analysis with projected CAM scores in 2035.

2. State of the art for screening of CAMs and integration of decision-making

The study enlisted most of the previous literature that performed screening of CAMs for battery cells, as shown in Table 1. The key terms used to identify the relevant literature include economic, environmental, toxicity, criticality and MCDM for screening CAMs suitable for batteries, specifically LIBs and SIBs. Consequently, it includes relevant methods and research focused on the broader CAM selection process. The literature review was conducted using major academic databases including Scopus, Wiley Online Library, ScienceDirect, Web of Science, and Google Scholar. The review includes the literature from 2018 to 2025.

3. Assessed chemistries of SIBs

The identification of promising CAM materials is based on previous studies, which address CAM comparisons regarding different aspects like energy density, cost, GHG, criticality, EOL-RIR, import reliability and toxicity.[5,12] In this study, a total of 23 SIB CAMs, both represented in ref. 5 and 12 are screened and compared with three state-of-the-art LIB technologies, specifically LFP, NMC 111 and NMC 622. Similar to LIBs, SIB CAMs can be categorised into layered oxides and polyanionic materials, which served as a categorization in this study. An overview of various CAM types with detailed insights into their properties is provided in Table 2. Most sources are based on lab-scale processes, which may differ from large-scale production methods. Solvents are not included in the analysis due to assumed recovery and lack of traceability, although they are mentioned in the results where possible.[5,12,13]

4. Evaluation criteria and data processing

Since material availability, cost and sustainability are key drivers in SIB development, a critical question is how to guide these efforts at an early stage, before technological advancements limit the potential to adopt a more sustainable solution.[25] In the early stages of technology development, such assessments are particularly important, as they enable adjustments to key factors that support the advancement of TRLs.[48] While the considered LIB chemistries have reached commercial maturity and broad mass application, some SIB chemistries remain at lower TRLs and are only beginning to enter initial testing and niche applications.

To support decision-making, it is necessary to apply flexible, easy to communicate and modular approaches based on appropriate selection criteria.[49] In this study, comprehensive evaluation criteria are considered in the screening method like cost estimation, energy density, import reliability, environmental footprint, EOL-RIR, raw material criticality and toxicity analysis, which can identify early-stage sustainability hotspots.[50] The values of energy density are derived from the literature (Baumann *et al.*, 2024[12]) due to limitations in experimental data availability. SR is used to assess material availability and is obtained from EU-based criticality assessment. Potential GWP impacts are based on the Environmental Footprint (EF) 3.0 methodology and ecoinvent 3.8 database. Material precursors including all upstream processes and material synthesis impacts are considered within the system boundary, with synthesis steps assumed to take place in Europe using an average electricity and heat mix. Infrastructure and auxiliary inputs are excluded due to limited data availability and their typically negligible contribution to overall CAM synthesis impacts.[5] More information on the system boundary can be found in the SI. The functional unit of this analysis is 1 kWh. Details on the used data can be found in Baumann *et al.*[5]

The hazard and input-related toxicity criteria are adopted from Baumann *et al.* (2024),[12] whereas cost, criticality and carbon footprint are based on Baumann *et al.* (2022).[5] Building on these complementary studies, the sustainability screening framework for CAMs is extended by integrating additional criteria, namely import reliability and EOL-RIR. Furthermore, all indicators (despite the GWP) are recalculated using an updated and harmonized dataset to ensure consistency and comparability. By integrating performance-related, economic, environmental, and hazard-related aspects within a unified framework, the resulting evaluation criteria enable a comprehensive and balanced screening of CAMs for both the LIBs and SIBs.[13] It is critical for strategic material selection, particularly at the early stages of development, where experimental data are limited. Details of the considered evaluation criteria are discussed in Table 3. The detailed calculation of the criteria is shown in Baumann *et al.* (2022)[5] and Baumann *et al.* (2024).[12]

The indicator value data are presented in Table 4.[5,12,13,25,51,52]

5. Methodologies

The study screens the CAMs for emerging batteries under different sustainability factors by using an HFL-MCDM approach. The detailed methodology of the proposed method is shown in Fig. 1.

Table 1 Literature review

Authors (year)	Objective	Methodology	Key findings	Limitations
Ellingsen *et al.* (2018)[22]	Evaluate technical and environmental impact of the AlCL3/EMIMCL electrolyte	Combination of different indicators, *e.g.* supply risk, power density and cycle efficiency	Each alternative has drawbacks	Economic and other detailed assessments are excluded
Potts *et al.* (2019)[23]	Evaluate technical properties of NCA and NMC	High-throughput electrochemical study	Study assessed different technical properties of batteries	Study focused on LIBs and evaluated technical parameters
Adhikari *et al.* (2020)[24]	Develop the synthesis method for SIB cathodes	High-throughput sol–gel	Highly stable Na–Fe–Mn–O cathodes synthesised	Only the technical performance is considered
Peters *et al.* (2021)[25]	Compared environmental impact of SIBs *vs.* LIBs	Full LCA	SIBs are promising, but Li performs better in some impact categories	Only a few environmental impacts are evaluated
Loganathan *et al.* (2021)[26]	Select LIBs for electric vehicles	MCDM	Lithium-titanate is optimal	Includes technical, economic, safety and reliability factors only
Baumann *et al.* (2022)[5]	Flexible CAM screening method	Cost, GHG and criticality hotspot	Most SIB CAMs show promising performance	Focused only on cost, GHG and criticality
Sayahpour *et al.* (2022)[27]	Summarise important CAM design	Literature and test data	• Prussian blue performs best • Higher energy density does not guarantee higher capacity retention	Analyzes only energy density and capacity
Rey *et al.* (2022)[28]	Environmental impact assessment of the $Na_3V_2(PO_4)_3$ cathode for SIBs	LCA	All cathodes show some level of toxicity	Only toxicity is evaluated
Lai *et al.* (2023)[29]	Carbon emission and environmental impact assessment of SIBs	LCA	Environmental impact of SIBs is lower than that of LIBs	Only environmental assessment is considered
Liang *et al.* (2023)[30]	Review different SIBs	Literature review	O3 layered oxide is identified as promising	Cost and environmental impact are considered
Baumann *et al.* (2024)[12]	Hazard and toxicity screening of CAMs	Hazard traffic light, total hazard point and LCA	Oxidic CAMs have high hazard scores, cyanide-based systems can pose a challenge	Focused only on energy density and hazard screening
Gutsch and Leker (2024)[31]	Cost and environmental impact assessment of LIB value chain (CAM synthesis)	Process-based cost model with LCA	• LIB cell costs: $94.5 per kWh • Global warming potential (GWP): 64.5 kg CO_2eq. per kWh • NMC 111 cost: $23 per kg, NMC 811: $21.5 per kg	Other factors like hazard, toxicity screening and criticality are not considered
Wang *et al.* (2024)[32]	Identify viable metal-ion battery alternatives to LIBs	Fuzzy best-worst method with combined compromise solution	SIBs and magnesium-ion (MIBs) most promising solution	Only the technical and economic factors are considered
Wanison *et al.* (2024)[33]	Examines engineering aspects influencing SIB electrode	Technical and economic comparison	Temperature management and high energy density with long cycle life are crucial	Only technical and economic aspects are considered
Das *et al.* (2025)[34]	Screen SIBs, potassium-ion and compare with LIBs	Fuzzy MCDM	LIBs are acceptable when all evaluation criteria are considered	Techno-economic, full LCA and socio-political factors are considered
Kim *et al.* (2025)[35]	To identify potential Li-rich metal oxide sacrificial cathodes	Computational synthesis	Li_6MnO_4 may be a potential option	Irreversible capacity is only determined

Table 2 Details of the considered CAMs

Property	Layered oxides[7,36–38]	Polyanionic materials/PBA[5,12,39–47]
Chemical formula	Na_xTMO_2 (TM = Mn, Fe, Ni, Co, Ti, *etc.*)	$Na_xTM_y(XO_4)_n$ (X = S, P, Si, As, Mo/W and TM = transitional material) • Developed with tetrahedron anionic units & polyhedral with strong covalent bonds • PBA: $Na_{2-x}TM_a[TM_b(CN_6)]_{1-y}\cdot zH_2O$
Energy density	High (100–260 Wh kg^{-1})	Moderate (120–220 Wh kg^{-1})
Cycle life	Up to 4000 depending on chemistry	Up to 6000 depending on chemistry
Working voltage	2.4–3.6 V	1.5–4.2 V
Structure pattern	Diffusion in prismatic layers: direct path octahedral layer: zigzag pattern	3D framework groups and transition metals are interconnected by strong covalent bonds
Number of transition metals	Number of TM layers per unit cell (denoted by numeral after P or O)	Includes Fe, Mn, V and Ti
Production complexity	Easy to produce and manufacture	More complex synthesis; energy intensive
Advantages	• High capacity and stability when combined with other TMs • Environmentally sustainable	• High redox potential (inductive effect) • High thermal stability, which makes them safer • Low electric conductivity • PBA: low-temperature synthesis, abundant materials, Fe most promising
Limitations	Moisture sensitivity	• Limited availability: poses supply risk • Structural stability and ionic conductivity may limit performance • Synthesis is energy intensive

Table 3 Evaluation criteria based on ref. 5,12,13,25,51,52; for details, refer to the SI

Factors	Sub-factors	Brief overview (relevant to battery CAM)	Equation/indicator	Calculation details
Technical	Energy density	It indicates how much energy a battery can store per unit mass or volume; higher values are desired for portable or automotive applications	$E_{vol} = E \times \rho_{cell}$ (1) $E_{grav} = \int V(Q)dQ$ (2)	Based on theoretical calculation without the anode
Economic	CAM cost	It reflects the material processing cost of the CAM; it is crucial for determining battery affordability and market competitiveness	$\text{Cost} = \sum(\text{material cost} \times \text{max fraction}) + \text{processing charge}$ (3)	Calculated based on the material shares and up-to-date material prices taken from SMM[52]
Raw material criticality and circularity	EOL-RIR	The criterion measures how much material can be recovered after recycling to support circularity and reduce raw material dependency	$\text{EOL-RIR}\ (\%) = \frac{\text{recycled input}}{\text{total material input}} \times 100$ (4)	Dimensionless value based on the average recycling rates of EU using ref. 53
	Supply risk (SR)	Indicates material supply disruption due to factors like trade policies, geographic concentration and market control	Indicates raw material criticality	Dimensionless value based on the average supply risk of EU using ref. 53
	Import reliability	Assesses geopolitical risk and supply reliability	Often expressed *via* a qualitative index	Dimensionless value based on average Import reliability of EU using ref. 53
Environmental	Carbon footprint	GHG emissions of the CAM are estimated based on an upstream process using the EF3.0 methodology	Important for environmental sustainability and assessed using ecoinvent V3.8 and OpenLCA	Only for precursor materials, does not include energy demand
Environmental/ "Social"	Environmental/ input-related human toxicity	Evaluates potential harmful effects of materials on human health and ecosystems	Important for safe production, use and disposal. Assessed through the total hazard point (THP) score	Calculation based on the THP score method[51]

The study, as illustrated in Fig. 1, introduces a hierarchical methodological framework to screen the CAMs of emerging batteries based on an overall sustainability factor. This assessment integrates major sustainability factors including technical, economic, environmental and social dimensions. Technical factors such as energy density, economic considerations like CAM cost,

Table 4 Indicator values[5,12,13,25,51]

Study		Energy density (Wh kg^{-1})	Supply risk (EU)	Economic importance [—]	EoL-RIR [—]	Import reliability [—]	Cost ($ per kWh)	Toxicity score (THP per kWh)	GHG (kg CO2 eq. kWh)	Projected CAM future cost in the year 2035
Layered oxide materials										
$LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$ (NMC 111)	A1	592	1.8	11.1	15.9	79.1	31.55	1674.00	42.4	105.56
$LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$ (NMC622)	A2	629	1.3	7.7	15.1	60.1	31.69	1466.00	34.6	62.9
α-$NaMnO_2$	A3	509	1.2	8.1	8.8	94.3	14.21	134.000	12	4.44
P2-$Na_{0.67}Mn_{0.95}Mg_{0.05}O_2$	A4	455	1.5	10.2	10.6	112.1	15.97	157	18.08	5.27
O3-$NaMn_{0.5}Fe_{0.5}O_2$	A5	303	1.4	9.8	33.3	143.1	22.86	155	14.4	2.55
O3-$NaNi_{0.5}Mn_{0.5}O_2$	A6	377	1.1	7.4	17.0	84.1	21.984	77.5	22.4	15.15
$Na[Mn_{0.4}Fe_{0.5}Ti_{0.1}]O_2$	A7	308	1.3	8.7	31.6	140.3	23.16	143	19.6	6.97
$NaMn_{0.33}Fe_{0.33}Ni_{0.33}O_2$	A8	481	0.8	5.1	19.7	70.8	14.64	1043	14.4	8.10
$Na_{0.6}Fe_{0.11}Mn_{0.66}Ni_{0.22}O_2$	A9	324	1.6	11.0	22.1	132.9	20.49	894	19.2	12.1
$NaMn_{0.3}Fe_{0.4}Ni_{0.3}O_2$	A10	390	0.9	6.1	25.8	88.6	17.42	59.6	22.6	9.03
P2-$Na_{0.6}Fe_{0.2}Mn_{0.65}Ni_{0.15}O_2$	A11	620	0.8	5.7	12.9	72.5	9.830	80.5	12	5.11
$Na_{0.6}Ni_{0.22}Al_{0.11}Mn_{0.66}O_2$	A12	675	0.8	5.4	9.5	61.3	9.9911913	444	12.2	6.04
Polyanionic materials										
$LiFePO_4$ (LFP)	A13	569	0.8	5.0	25.2	82.5	23.43	301	11.7	28.7
$Na_3V_2(PO_4)_3$	A14	381	1.9	8.7	12.6	102.6	41.24	250	46.8	12.16
$Na_{1.702}Fe_3(PO_4)_3$	A15	406	0.9	6.0	33.9	102.8	25.71	113.3	11.2	0.7
Na_2MnPO_4F [a]	A16	651	0.8	5.2	7.4	64.0	16.58	35.8	8.4	2.03
$Na_2MnFe(CN)_6$ [a]	A17	490	0.6	4.3	14.5	62.5	22.11	11.9	9.6	2.61
$Na_{0.61}Fe[Fe(CN)_6]_{0.94}$ [c]	A18	493	0.6	4.2	35.8	89.0	21.37	2.9	9.4	1.71
$Na_{0.81}Fe[Fe(CN)_6]_{0.79}$ [c]	A19	447	0.5	3.3	28.7	71.2	23.59	3.1	9.6	1.28
Na_2FeSiO_4 [a]	A20	724	0.5	2.7	12.3	42.6	15.09	53.64	6.4	1.66
Na_2MnSiO_4 [a]	A21	630	0.8	5.2	4.1	57.2	17.89	83.44	7.84	3.58
$NaFePO_4$	A22	410	0.8	5.6	31.7	96.0	25.48	23.84	9.6	0.66
$Na_4MnV(PO_4)_3$	A23	380	1.5	8.2	13.0	98.1	34.39	286.1	28.4	7.56
$Na_3MnTi(PO_4)_3$ [a]	A24	410	1.0	6.3	11.3	94.4	27.35	65.56	14.2	7.73
$Na_3MnTi(PO_4)_3$ [b]	A25	506	0.8	5.1	9.2	76.5	22.16	95.36	11.8	6.26
$Na_3MnZr(PO_4)_3$		402	1.2	6.5	15.8	109.5	26.68	26.82	12	3.51

[—] – indicates the dimensionless indicator. [a] 2Na exchange. [b] 3Na exchange. [c] Prussian blue analogues.

environmental indicators such as carbon footprint, and raw material criticality indicators like SR, EOL-RIR and import reliability are considered. Hazard and toxicity screening are also evaluated as part of the sustainability criteria for CAM selection. The criteria are selected based on two previous studies by Baumann *et al.*,[5,12] with the cost and criticality revised and recalculated based on the most recent data available. Additional criteria, including EOL-RIR, economic importance and import reliability have been included in this study[53] (see the SI for details on the calculation and normalization). These factors often conflict with each other and linguistic uncertainty poses complexity and significant uncertainty in decision-making. To address these challenges, this study employs a hybrid HFL-MCDM approach. Specifically, the HFL-AHP is used to assign weights to the criteria, while the NEAT-Fuzzy-PROMETHEE method is applied to rank the alternatives.

Initially, the study evaluates the ranking of the alternatives on the basis of techno-economic, environmental and other factors. In the next step, the hazard and toxicity criteria are introduced with the other evaluated criteria to check the impact of the toxicity factor in decision-making. Additionally, a novel obstacle degree model is proposed to identify and quantify barriers posed by specific criteria that may hinder the selection of optimal storage technologies. This model highlights potential hotspots and supports a thorough analysis of how variations in input parameters affect decision outcomes. A comprehensive sensitivity analysis is conducted. Lastly, the study includes a prediction of future CAM costs for the year 2035, to examine how changes in cost affect the ranking of alternatives. This enables a future oriented evolution of CAMs. The applied methods of this study are discussed in the following sections.

5.1. HFL-MCDM method

Hesitant fuzzy multi-criteria decision-making, proposed by V. Torra, is based on the comparative Hesitant Fuzzy Linguistic Term Set (HFLTS) and is well-suited to handle situations with hesitation and limited information.[54] According to this method, the membership function values can take multiple possible options within the range [0,1]. This flexibility allows for the explicit representation of hesitation in the assessment process, making it a robust tool for managing high levels of uncertainty. Later, Liu and Rodríguez extended this concept by developing an MCDM model in which decision-makers can express their evaluations using linguistic expressions derived from HFLTS.[55] It further enhances the applicability of hesitant fuzzy methods in uncertain decision environments. Decision-makers implement language terms that are comparable with HFLTS for assessing the criteria and alternatives. This method offers both actual and linguistic expression versatility to overcome doubt and hesitation.[56] The details of this HFL method are discussed in the SI (section A.3).

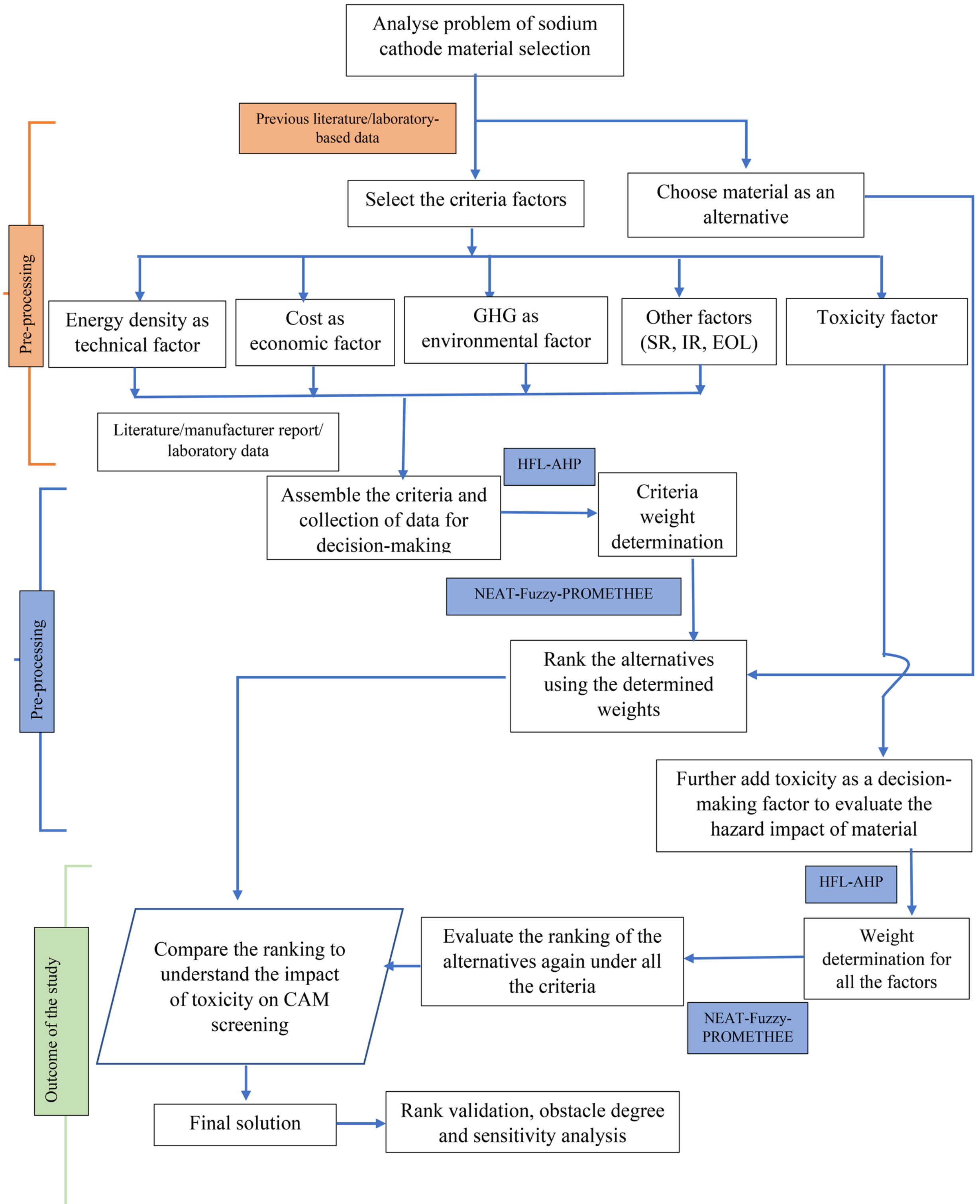


Fig. 1 Hierarchical methodology.

The study considered two different MCDM approaches for weight determination and ranking analysis. The HFL-AHP is used to decide the criteria weights[57] and the intuitionistic NEAT-Fuzzy-PROMETHEE approach is considered for the ranking evolution. Decision-makers often experience cognitive uncertainty, and fuzzy expressions are preferred for assessments. However, when inconsistencies arise such as when decision-makers express scores in ranges (*e.g.*, "between 6 and 8") rather than precise values (*e.g.*, "7"), the use of HFL-AHP becomes necessary.[58] The advantages of these two methods are discussed in ref. 34 and 59.

The HFL-AHP method was first introduced by Saaty and is most widely used in decision-making to date.[57] The process involves conducting pairwise comparisons among criteria and alternatives.[60] The consistency of pairwise comparison matrices, in which decision-makers assign scores, is evaluated to ensure reliability. The steps followed in this method are discussed in Fig. 2. The scaling is shown in Table 5[61] and the scale is developed using triangular fuzzy number (TFN).[62,63]

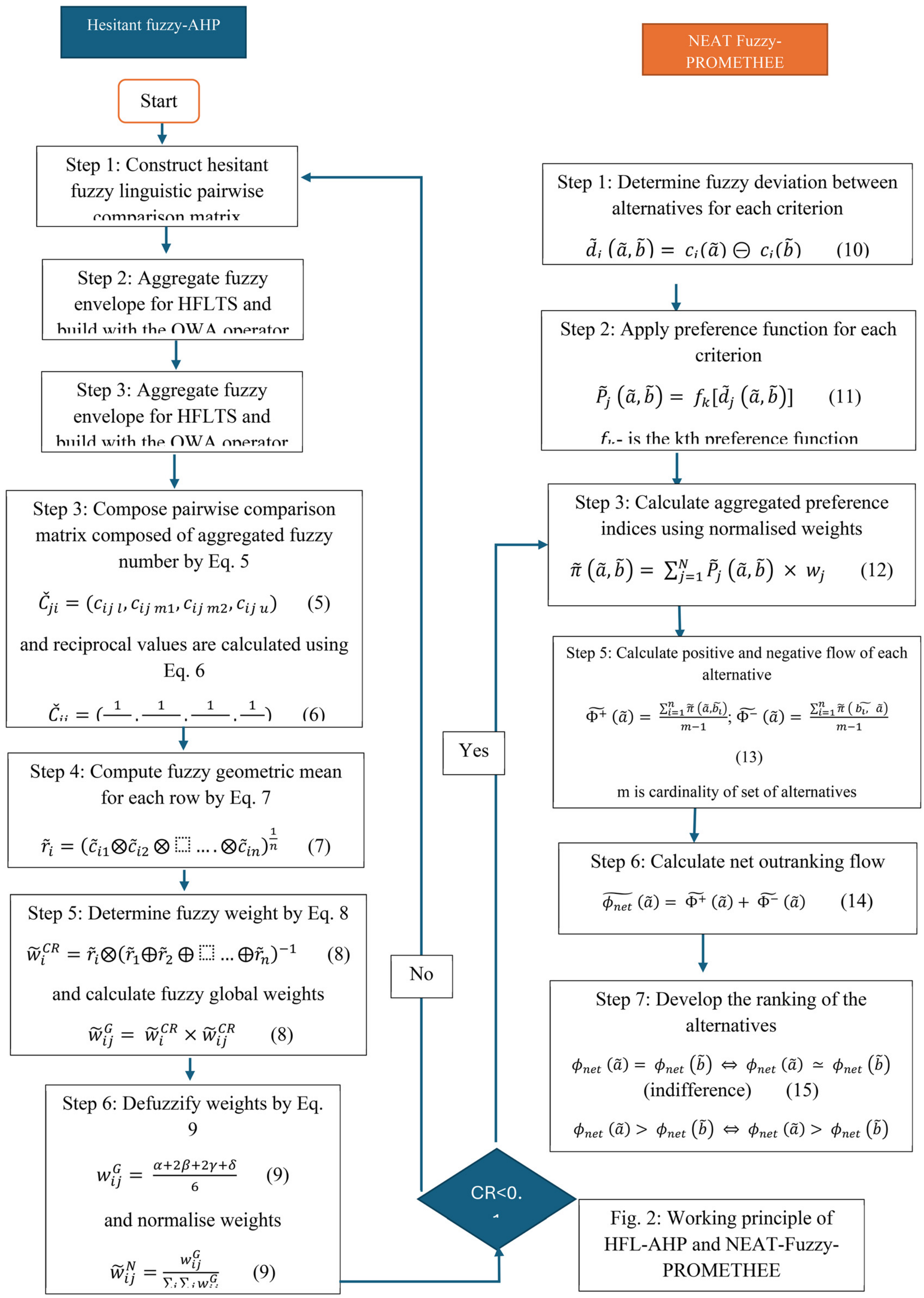


Fig. 2 Working principle of HFL-AHP and NEAT-Fuzzy-PROMETHEE.

Table 5 Linguistic scale of HFL-AHP for weight calculation [61]

Linguistic term	Abb.	TFN
Definitely high importance	DHI	(7, 9, 9)
Extremely high importance	EXHI	(5, 7, 9)
Essentially high importance	ESHI	(3, 5, 7)
Weakly high importance	WHI	(1, 3, 5)
Equally high importance	EHI	(1, 1, 3)
Exactly low importance	EE	(1, 1, 1)
Equally low importance	ELI	(1/3, 1, 1)
Weakly low importance	WLI	(1/5, 1/3, 1)
Essentially low importance	ESLI	(1/7, 1/5, 1/3)
Extremely low importance	EXLI	(1/9, 1/7, 1/5)
Definitely low importance	DLI	(1/9, 1/9, 1/7)

Another method, the NEAT-Fuzzy-PROMETHEE method, is used to evaluate the rank of the alternatives by using the estimated weights of the criteria.[64] This method is the new intuitionistic decision-making approach developed by P. Ziemba.[65] The trapezoidal fuzzy number (TrFN) scale is used which allows the use of the natural fuzzy criteria values along with the linguistic scales shown in Table 6.[66] This method includes two steps. The NEAT-Fuzzy-PROMETHEE 1 method provides a partial order of the alternatives and the NEAT-Fuzzy-PROMETHEE 2 method gives a final order of the alternatives in both crisp and fuzzy form.[67] Fig. 2 demonstrates the equations that are used to develop the working principle of this method.

5.2. Obstacle degree method

To comprehensively explore the contribution of each criterion to the overall obstacle degree of each alternative and to analyse the relationships among criteria, the methodology of obstacle degree analysis and correlation matrix of criteria is introduced. These evaluations will identify the obstacles that constrain the recognition of sustainable CAM, which is in line with the EU's Sustainable Development Goals (SDGs). These factors are based on the evaluation criteria of each battery's CAM screening process. The obstacle degree is calculated using eqn (15) and (16).[68,69]

$$P_{ij} = 1 - V_{ij} \tag{15}$$

$$O_j = \frac{P_{ij} \times W_i}{\sum_{i=1}^{m} P_{ij} \times W_i} \times 100\% \tag{16}$$

where O_j is the obstacle degree of the i^{th} indicator, P_{ij} is the degree of deviation for the i^{th} indicator and W_i is the factor's weight.

With the degree of obstacle analysis, the study evaluates the interdependencies of the criteria through a correlation matrix. It is important to identify interdependencies among criteria, ensuring that each factor provides distinct information and contributes meaningfully to the analysis. To calculate this correlation, the dataset is prepared by compiling the numerical values of the criteria for each of the CAM alternatives. These values are organised in a criteria matrix in which row represents an alternative and column corresponds to each criterion. This structured matrix is then used as the input for computing the pairwise correlation between the criteria through Pearson correlation analysis. This analysis helps to identify possible interdependencies and overlapping information among the criteria.[70]

5.3. Sensitivity analysis

The sensitivity analysis aims to validate the outcome of the analysis to evaluate the robustness of the proposed methodology. To validate the criteria weights, which are obtained through a fuzzy subjective weighting method, the study introduces an objective weight determination approach followed by the hybrid objective subjective MCDM method. The hybrid approach balances both the objective and subjective weights and then provides a normalised weight. The HFL-TOPSIS method is then included to validate the ranking of alternatives under the obtained weight of the criteria. Furthermore, this sensitivity analysis includes an evaluation that examines the ranking of alternatives under the projected CAM cost to assess how the change in material cost can influence the final decision. This comprehensive sensitivity assessment will help to obtain a robust solution.

5.3.1. CRITIC-OSWMI method. The study considered the hybrid OSWMI MCDM method followed by the CRITIC method as a common objective approach. This is to validate the criteria weights initially derived using the HFL-AHP method. Under the objective method, CRITIC is widely used and considers both contrast intensity and inter-criteria conflict.[71] This makes the method more comprehensive and adaptable. The CRITIC method is applied in various domains such as biped robot control, ceramic tool design, *etc.*[72] However, this method may assign excessively high weights to criteria with high conflict or contrasts. It potentially allows a few criteria to dominate the decision-making process. It reduces the influence of such dominant criteria, without changing the overall ranking, and can improve decision balance.[73]

Table 6 Linguistic scale in NEAT-Fuzzy-PROMETHEE[65,66]

Weight of the criteria		Alternative ranking	
Linguistic scale	TrFNW = ($w1$, $w2$, $w3$, $w4$)	Linguistic scale	TrFNA ($a1$, $a2$, $a3$, $a4$)
Very low	(0,0, 0.1, 0.2)	Very poor	(0, 0, 1, 2)
Low	(0.1, 0.2, 0.2, 0.3)	Poor	(1, 2, 2, 3)
Medium low	(0.2, 0.3, 0.4, 0.5)	Medium poor	(2, 3, 4, 5)
Medium	(0.4, 0.5, 0.5, 0.6)	Fair	(4, 5, 5, 6)
Medium high	(0.5, 0.6, 0.7, 0.8)	Medium good	(5, 6, 7, 8)
High	(0.7, 0.8, 0.8, 0.9)	Good	(7, 8, 8, 9)
Very high	(0.8, 0.9, 1, 1)	Very good	(8, 9, 10, 10)

The theoretical concept of the proposed objective–subjective weighted method for minimising inconsistency (OSWMI) is discussed in this section. It is presented in four phases:[74]

1. Normalising the performance ratings of the alternatives for different evaluation criteria
2. Evaluating the CRITIC weight of the criteria
3. Considering the HFL-AHP method weights
4. Integrating the HFL-AHP weight and CRITIC weight for the final outcome

5.3.2. HFL-TOPSIS. The obtained ranking of alternatives is validated by the HFL-TOPSIS method. This is an updated version of TOPSIS method, which was first proposed by Hwang and Yoon as discussed in kilic and Kaya, (2015).[75] The advantages of this MCDM approach is discussed in Das *et al.* (2025).[34] The working principle is shown in section A.4 of the SI.

5.3.3. Future-oriented ranking evaluation under projected CAM costs. Along with the weight and rank validation, the study investigates how variations in projected CAM costs affect the ranking of the alternatives. It introduces a future-oriented sensitivity framework to assess the impact of anticipated CAM cost changes. This framework evaluates how projected cost variations by 2035 may influence the selection of viable CAM solutions. This step enables the evaluation of ranking stability and highlights whether criteria such as CAM costs exert a dominant influence on the final outcome. Such insights are valuable for ensuring balanced and robust decision-making under future uncertainty.[12]

6. Results and discussion

This study aims to screen CAMs for SIBs based on a comprehensive set of sustainability criteria, including techno-economic and socio-environmental dimensions. The initial stage of the evaluation uses criteria such as cost, energy density, GHG, cycle life, ROL-RIR, import reliability and criticality. In the next step, toxicity and hazard are added to the evaluation criteria alongside the others. This allows the analysis to observe how their inclusion influences the ranking and brings greater focus to environmental concerns. Inclusion of toxicity into the evaluation supports more informed and responsible decision-making by accounting for long-term regulatory and environmental implications. It is particularly important under the evolving EU chemical safety regulations and sustainability framework, which increasingly influence material acceptability and lifecycle compliance. Comparing results with and without this criterion provides deeper insights into their relative impact on decision-making, helping to balance the technical development and sustainability. However, with the integration of more criteria, the decision-making becomes complex and includes more uncertainty. Therefore, to overcome this limitation, an integrated hesitant fuzzy-intuitionistic MCDM approach is employed to evaluate and rank the alternatives according to the defined criteria. Additionally, the study includes an obstacle degree analysis, assesses the potential impact of future cost growths, and validates the robustness of criteria weights and material rankings. A detailed discussion of these analyses is presented in this section.

6.1. Weight determination and ranking analysis (without toxicity)

In this phase, the HFL-AHP method evaluates the weights of the techno-economic and environmental criteria including energy density, cost, GHG, economic importance, EOL-RIR and import reliability. The result is shown in Fig. 3 and the detailed evaluation result is shown in Table 7.

The weight assessment shows that energy density and cost emerged as the most influential factors, each contributing approximately 20.8% to the overall decision-making process. These values are closely followed by GHG, which holds a weight of about 19.8%. Other factors like SR and economic importance account for roughly 12.4% and 10.4% of the total weight, respectively. End-of-life recyclability and import reliability represent smaller shares of the total weight, at approximately 8.6% and 7.3%, respectively. This distribution highlights the emphasis placed on performance and economic feasibility, while acknowledging environmental and resource-related concerns. The CR value shown in Table 7 is within the acceptable limit which justifies the developed pairwise matrix and the estimated weights of the criteria.

Considering this weight, the ranking analysis is carried out, and the assessment result is shown in Fig. 4a and b.

The fuzzy outranking flow and partial order assessment result show a comprehensive ranking of the CAMs for SIBs. Alternatives A20 and A12, corresponding to Na_2FeSiO_4 and $Na_{0.6}Ni_{0.22}Al_{0.11}Mn_{0.66}O_2$, respectively, are ranked first and second due to their balanced performance across techno-economic and emission criteria. Alternative A20 (Na_2FeSiO_4) secures the top rank owing to its low-cost synthesis, high energy density, Earth abundant elements and strong structural stability. These align well with sustainability metrics like low economic and environmental impact with high technical performance. Alternative A12 ($Na_{0.6}Ni_{0.22}Al_{0.11}Mn_{0.66}O_2$) ranks second, benefiting from moderate energy density and

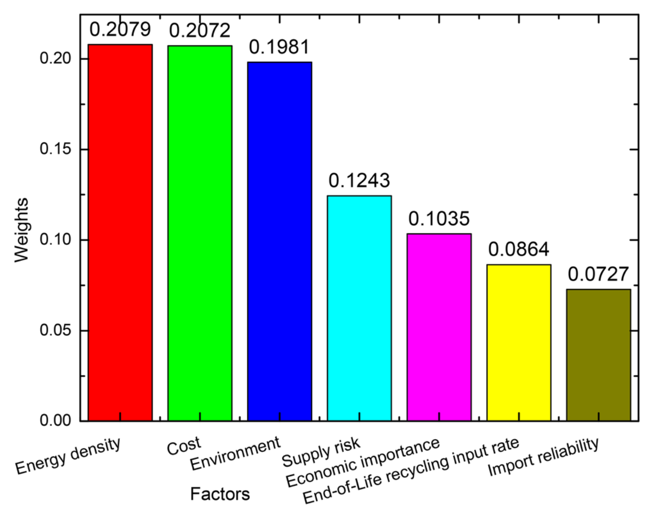
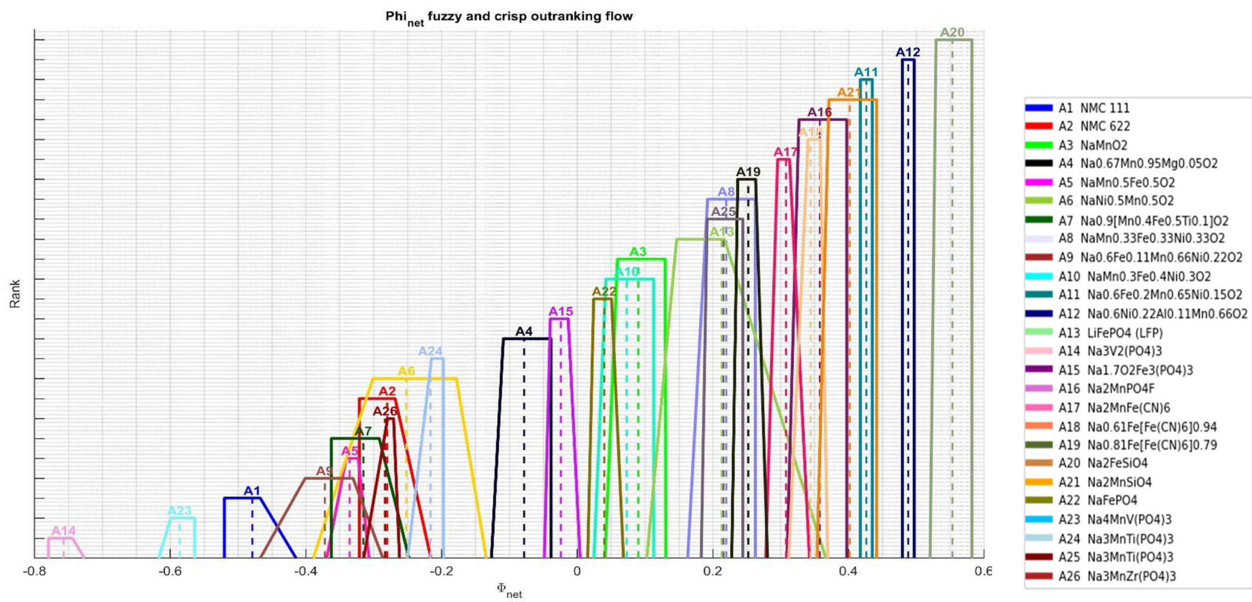


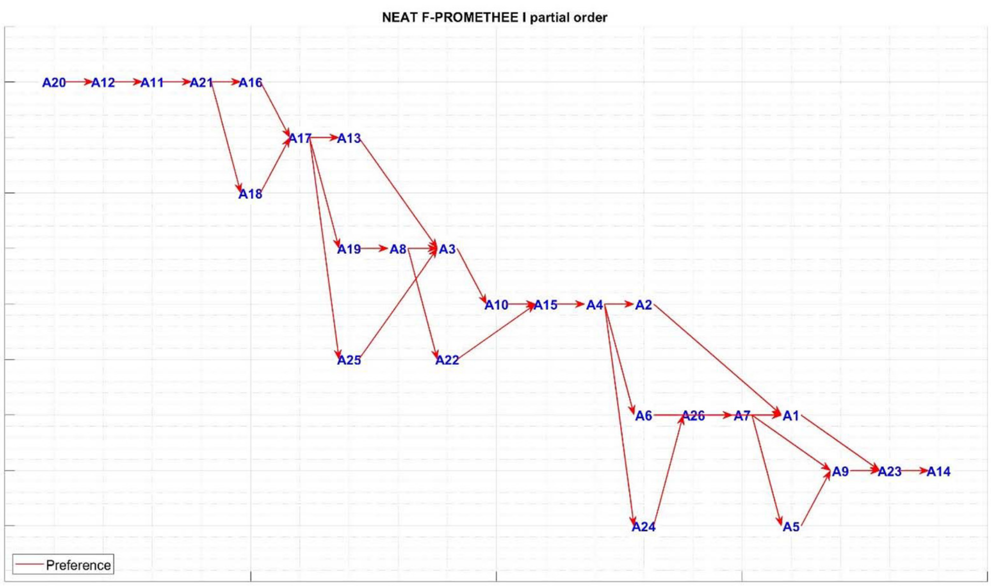
Fig. 3 Weights of the criteria.

Table 7 Weights and consistency ratio

	Factors					
Indicator	CW	WSV	Λmax	CI	CR	CR < 0.1
Energy density	0.1841	1.5942	7.7303	0.1217	0.0902	True (acceptable)
Cost	0.1841	1.5212				
Environment	0.1731	1.4631				
Supply risk	0.1381	1.0423				
EI	0.1224	0.7763				
EOL-RIR	0.1072	0.6432				
IR	0.0908	0.6093				



(a)



(b)

Fig. 4 Ranking of alternatives: (a) net outranking result and (b) partial order.

improved cycling stability due to Al doping. However, its Ni content introduces moderate cost and environmental concerns. In contrast, commercially available CAMs such as NMC 111 (A1) and NMC 622 (A2) rank significantly lower, as shown in their negative outranking flow values. Though they show high energy density, the presence of elements like Ni and Co increases the cost and emissions along with poor SRs. The analysis confirms that emerging, simple composition, and environmentally benign sodium-ion cathodes are more optimal choices over others. The corresponding crisp values are shown in Table A.2 of the SI.

In the next step, the study includes the hazard and toxicity factor with the other assessment criteria to comprehensively screen the CAMs.

6.2. Weight and ranking analysis with toxicity

The weight determination of the overall criteria is shown in Fig. 5, and the detailed description of this evaluation is shown in Table 8.

Fig. 5 ranks energy density (0.1853), cost (0.1846) and GHG emissions (0.1772) as the most impactful factors. These factors collectively account for just over 54% of the total decision weight, underscoring a clear preference for higher technical performance, economic viability and environmental impact in material selection decisions. Factors such as SR, economic importance and end-of-life recyclability together contribute 28%, which indicates moderate concern for resource criticality and circular economy practices. Interestingly, this weight evaluation indicates that toxicity has a weight of 10.71% of the total, positioning it higher than factors like import reliability. This indicates growing awareness of health and safety considerations in material life cycle assessment. While toxicity is not among the top three, its notable share highlights its non-negligible role, specifically in contexts where regulatory compliance and human-environmental safety are critical. The overall consistency ratio of under 0.1 confirms the logical coherence of the assigned priorities (Table 8).

The ranking analysis is further carried out with these criteria weight, and the analysis result is shown in Fig. 6a and b.

In Fig. 6a, the net outranking flow provides the rank of the alternatives across multiple criteria, and Fig. 6b provides a partial order of preferences among alternatives. Among the alternatives, A18 ($Na_{0.61}Fe[Fe(CN)_6]_{0.94}$) achieves the highest position with the most positive net flow. The superior performance is attributed to its balance across different key criteria, including cost, environmental impact and toxicity. It has also moderately high energy density. Unlike Co and Ni-based materials, A18 uses abundant, low-cost and environmentally benign elements like sodium and iron. Its PBA structure enables good electrochemistry, stability and high rate capability, which lead to a favourable energy density. Furthermore, its non-toxic composition gives it a distinct edge in the decision-making framework, where toxicity is given a notable weight in the analysis. Similar to the previous analysis result, the commercially available CAMs like NMC 111 (A1), NMC 622 (A2) and $Na_3V_2(PO_4)_3$ (A14) are placed at the lower end of the ranking due to unfavourable characteristics like high cost, poor environmental compatibility and increased toxicity from elements like cobalt, vanadium and nickel.

The partial order graph also validates the ranking by showing A18's dominance through consistent preferential paths over other alternatives. Materials like A13 (LFP) and A12 ($Na_{0.6}Ni_{0.22}Al_{0.11}Mn_{0.66}O_2$) obtain the middle range due to their moderate sustainability performance. Overall, this analysis indicates a clear transition in materials preference, favouring safer, more sustainable and economic options like

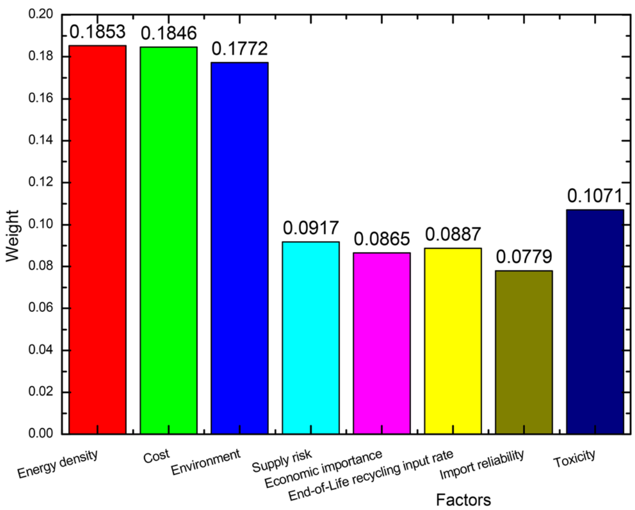
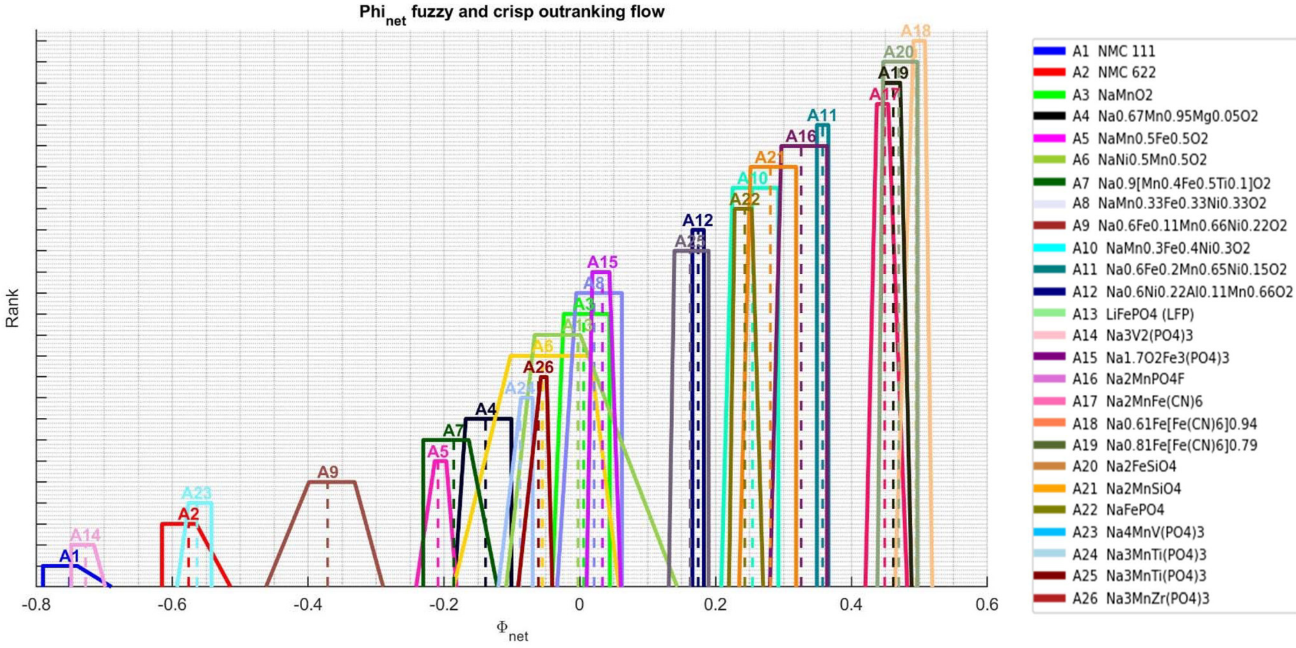


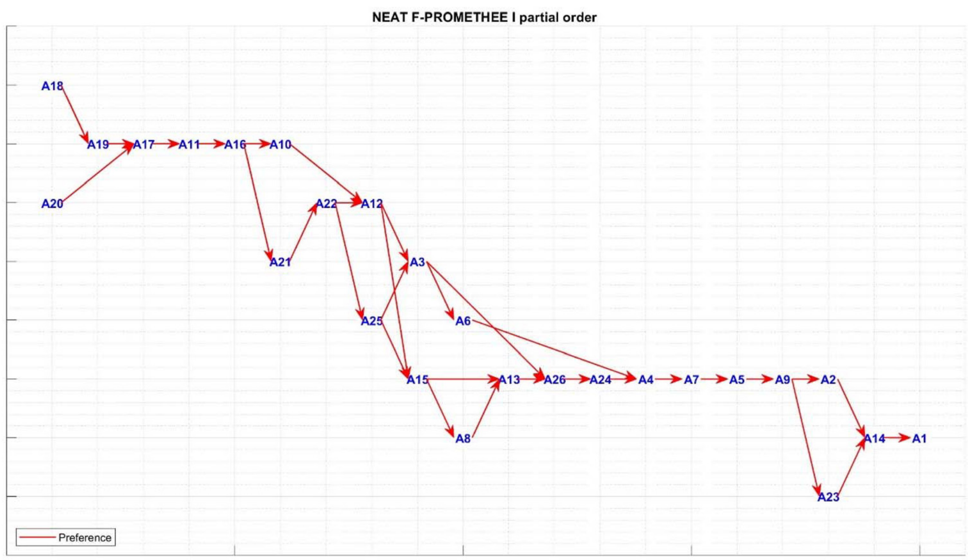
Fig. 5 Weights of the overall criteria.

Table 8 Weights and consistency ratio

	Factors					
Indicator	CW	WSV	Λmax	CI	CR	CR < 0.1
Energy density	0.159	1.6071	8.9594	0.1371	0.0979	True (acceptable)
Cost	0.157	1.5411				
Environment	0.151	1.4902				
Supply risk	0.119	1.0361				
EI	0.106	0.8092				
EOL-RIR	0.103	0.7152				
IR	0.094	0.6793				
Toxicity	0.105	0.9563				



(a)



(b)

Fig. 6 Ranking analysis: (a) net outranking flow and (b) partial order analysis.

A18 over conventionally high energy but less sustainable alternatives. The crisp values are found in Table A.3 of the SI.

The findings of this study are consistent with previous works by Baumann *et al.* (2022)[5] and Baumann *et al.* (2024),[12] which also identify Prussian blue analogues (PBAs) as promising candidates from techno-economic and socio-environmental perspectives. It is worth mentioning that results for PBA in terms of hazards and toxicity can shift significantly if notification thresholds for the THP method are changed. However, those studies assessed the criteria separately. In contrast, the present study integrates and extends these criteria by incorporating additional factors such as supply risk (SR), import reliability, and EOL-RIR. This comprehensive and integrated assessment framework enhances the robustness of the analysis and further supports the validity of the results when compared with previous studies.

6.3. Degree of obstruction analysis

The proposed degree of obstruction identifies the extent to which each criterion limits the overall performance of the alternatives and the evaluation result is shown in Fig. 7. The criteria interdependency analysis shown in Fig. 8 provides insight into whether improvements in one attribute may positively or negatively affect others. Thus, this overall analysis highlights the potential bottlenecks in material selection.

Fig. 7 clearly depicts that alternatives A1 and A2 suffer the highest total obstacle contribution, predominantly driven by toxicity, which accounts for 65–70% of the total obstacle. This

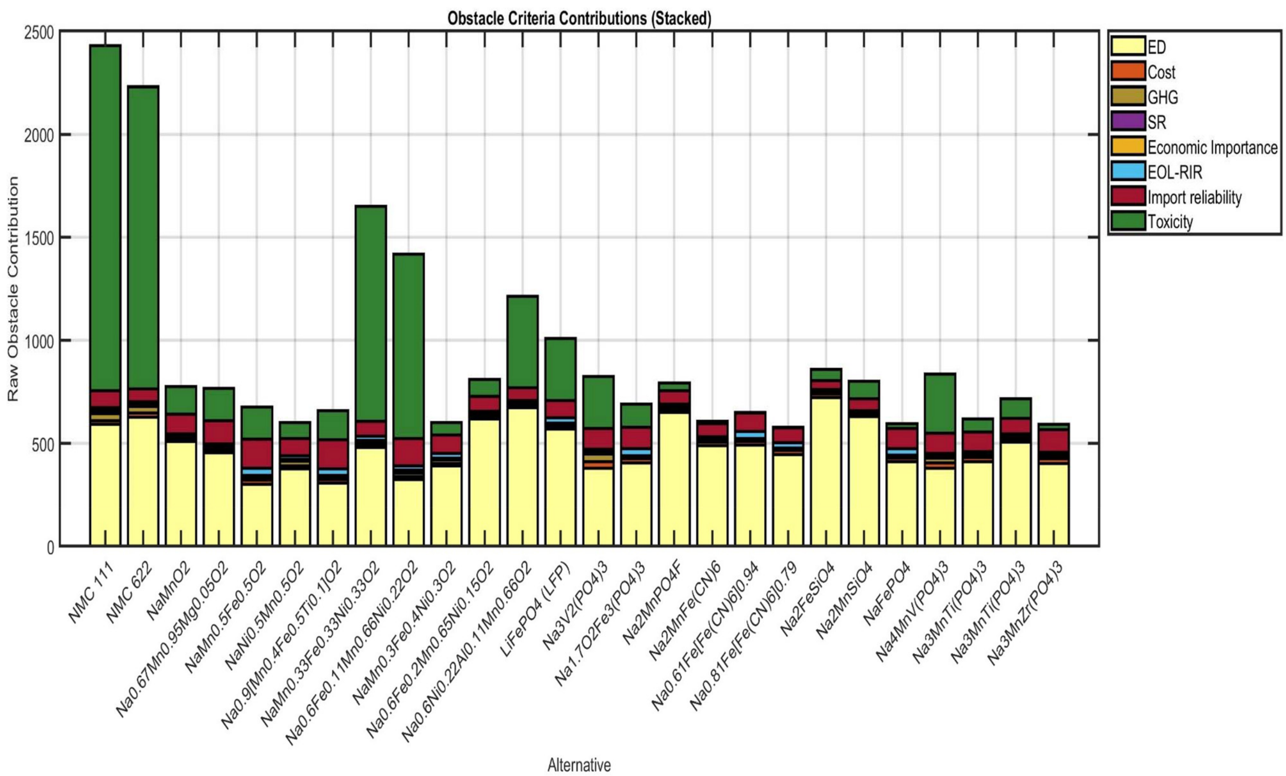


Fig. 7 Obstacle degree analysis.

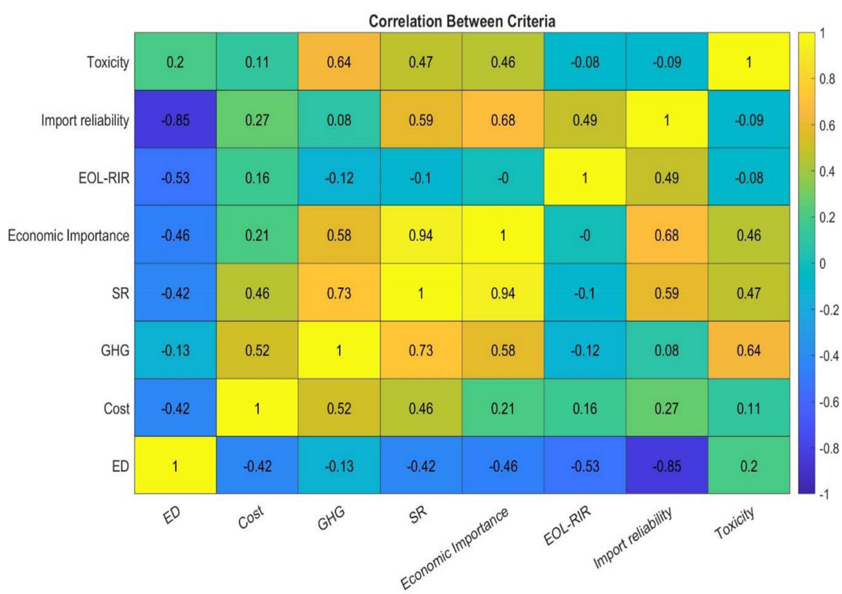


Fig. 8 Criteria correlation.

suggests that despite other advantages, it severely hinders practical adoption due to health and environmental concerns related to material toxicity. Energy density also consistently contributes a significant amount across all alternatives, specifically forming 50–55% of the total obstacle load, mostly in mid- to lower ranking options. This suggests that the lower technical performance is a major barrier regardless of alternatives, and improving energy density would universally enhance the performance of the material. From the analysis, it is noted that criteria like import reliability and GHG emissions are present across all alternatives in a modest amount, indicating that they are secondary yet non-negligible barriers. Alternatives like A7, A9 and A13 also show high contributions from toxicity and import reliability, reinforcing how a combination of environmental and geopolitical SRs intensifies the challenge. Conversely, alternatives like A16, A18 and A19 present lower cumulative obstacles and more balanced trade-offs, which implies that these are the most viable options. Additionally, this analysis justifies that reducing toxicity and improving energy density followed by cost, GHG emissions and import reliability should be primary targets to lower barriers across all the alternatives. This obstacle degree analysis shows the improvement region beside the ranking of the alternatives.

Fig. 8 shows that the strongest positive correlation is between SR and economic importance at 94%, indicating that materials that are considered economically important are also highly vulnerable to SR. This suggests that critical materials for the economy are often the least secure. Similarly, the GHG shows strong positive correlations with SR (73%) and toxicity (64%), which implies that materials with higher GHG emissions are also more toxic and pose greater supply challenges. On the other hand, energy density is negatively correlated with import reliability (−85%), which suggests that as the energy density improves, the reliance on imported materials decreases significantly. This is an important insight for reducing geopolitical vulnerability. Other notable findings include the moderate 52% correlation between cost and GHG, which suggests that more expensive materials often emit more GHGs, possibly due to complex manufacturing processes. Furthermore, based on these detailed correlation insights, the obstacle degree analysis is performed, which indicates the most critical barriers.

6.4. Sensitivity analysis

The study includes a comprehensive sensitivity analysis to validate the robustness of the results. This analysis addresses both the criteria weighting and the ranking of the alternatives.

To validate the criteria weights, both objective and subjective methods are employed. Specifically, the study includes the OSWMI method, which is the hybridisation of the objective and subjective MCDM methods. The HFL-AHP is the subjective MCDM approach, and in this study, the CRITIC MCDM approach is considered as an objective MCDM approach. The OSWMI method effectively balances these two inputs and ensures a more reliable and balanced weighting scheme. The ranking of the alternatives is then validated using the HFL-TOPSIS method, reinforcing the consistency and credibility of the final outcomes.

6.4.1. Weightage validation. The result of the CRITIC and OSWMI methods is shown in Fig. 9 and 10, respectively.

The assessed criteria weights from OSWMI (Fig. 10) considered both the weights of CRITIC (Fig. 9) and the HFL-AHP method. This hybrid approach balances both the objective and subjective methods and the result indicates that cost holds the highest priority of 21.5%, followed by GHG emissions (18.6%) and energy density (17.1%). The toxicity criteria also show high priority with 12.5% of the total weight. The trend of this assessment is aligned with the outcome of CRITIC (cost: 23.2%, GHG: 18.1% and SE: 16.4%). This sensitivity analysis validates that the weights obtained through the HFL-AHP method are robust. The ranking validation is then done by using the obtained weights.

6.4.2. Ranking validation. The ranking validation is conducted using the HFL-TOPSIS method, applying both CRITIC and OSWMI weights. The closeness coefficient and the corresponding ranking of the alternatives for each weighting method are shown in Fig. 11.

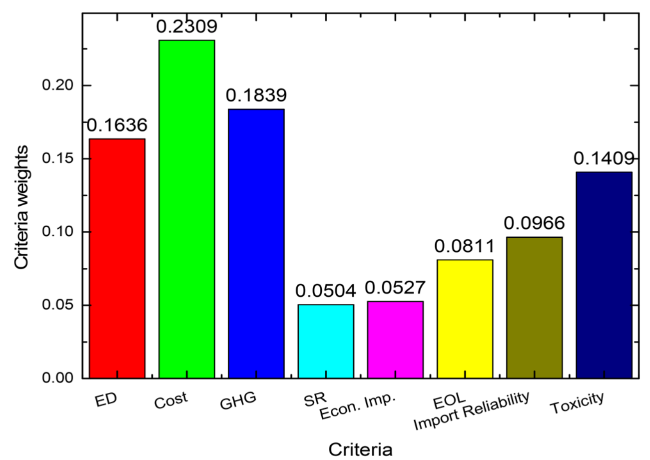


Fig. 9 Criteria weights by the CRITIC method.

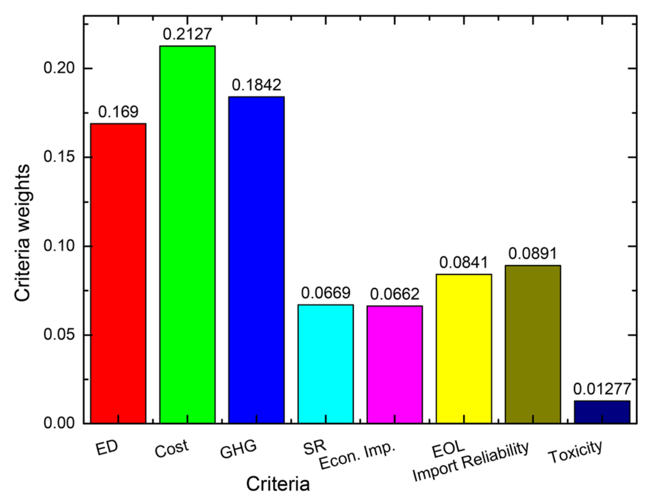


Fig. 10 Criteria weights by the OSWMI method.

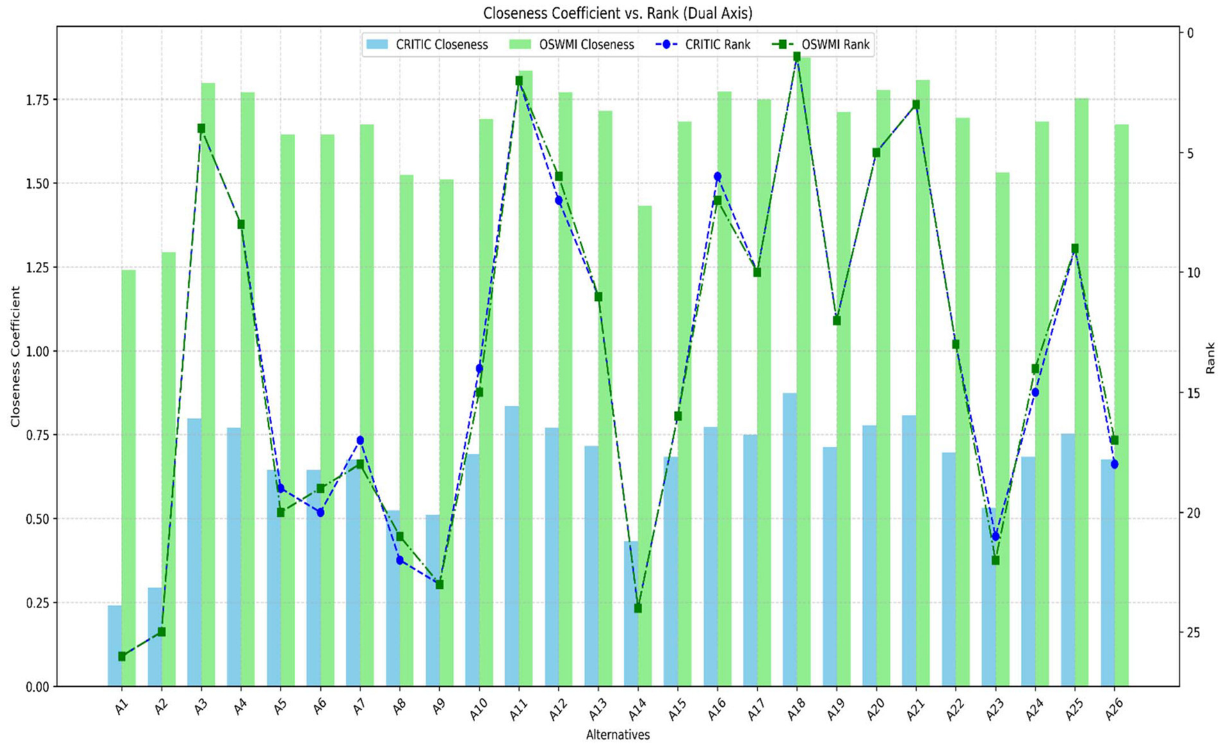


Fig. 11 Ranking of alternatives using HFL-TOPSIS.

According to the analysis, a high degree of consistency is observed, specifically in the top and bottom ranked alternatives. It is observed that alternative A18 is consistently ranked first under both weighting schemes, and A11, A20 and A21 also remain within the top rank across the methods. This indicates that these alternatives are the most favourable options. Similarly, A1 and A2 consistently appear at the bottom, reinforcing their lower performance under some criteria. Minor rank shifts are observed, as between A5 and A6 or A16 and A12. This is mostly because of the inherent differences between the CRITIC and OSWMI methods. This small deviation highlights the sensitivity of middle range alternatives but does not significantly affect the overall decision reliability. The top and bottom rankings are consistent across both methods. The assessment result validates that the previous solution are well aligned. This reinforces the robustness of the evaluation and validates the final outcome produced by the NEAT-Fuzzy-PROMETHEE methods.

6.4.3. Effects of projected CAM cost of 2035 on CAM rankings. The projected CAM cost evaluation for 2035 is conducted to assess the potential impact of future economic growth on material prioritisation. This sensitivity analysis supports a forward-looking understanding of cost-driven shifts in CAM selection under evolving market conditions. The assessment result is shown in Fig. 12. Fig. 12a and b present the net ranking and the partial order rank of the alternatives, respectively.

According to the assessment, it is observed that the projected future CAM cost by 2035 has a significant impact on the selection of alternatives. The ranking of the alternatives varies under this condition, with Na_2FeSiO_4 emerging as the highest ranked alternative, followed by $Na_{0.61}Fe[Fe(CN)_6]_{0.94}$. Again, the results for $Na_{0.61}Fe[Fe(CN)_6]_{0.94}$ can change if the method for THP is adjusted.[12] However, the cost of this CAM is projected to increase, but considering the growth of other CAM costs, the increment rate is lower. This makes it a more favourable solution than the previously top ranked alternative A18. However, changes in CAM costs also cause shifts among lower-ranked alternatives. For instance, alternative A2 moves to a mid-range position, while A14 becomes the lowest accepted alternative.

Therefore, production capacity growth and the associated cost reductions in CAM play a crucial role in reshaping the priority and feasibility of the alternatives. This highlights the dynamic nature of the proposed decision-making approach, where changes in material costs can elevate the attractiveness of certain alternatives while lowering others. This ultimately affects overall decision-making to select the best option, and this assessment makes the analysis more comprehensive.

6.4.4. Parameter variation impact. The results are highly dependent on the used energy density, which is based on theoretical values of the CAM. In the assessment, energy density values without the anode are calculated to make all the different CAMs comparable. However, energy density has, as explained before, a high impact on the other indicators. The effect is the same for all considered indicators, and is provided for the GWP and SR. This sensitivity can be seen in Fig. 13 using three higher ranked CAMs for LFP, $Na_{0.61}Fe[Fe$

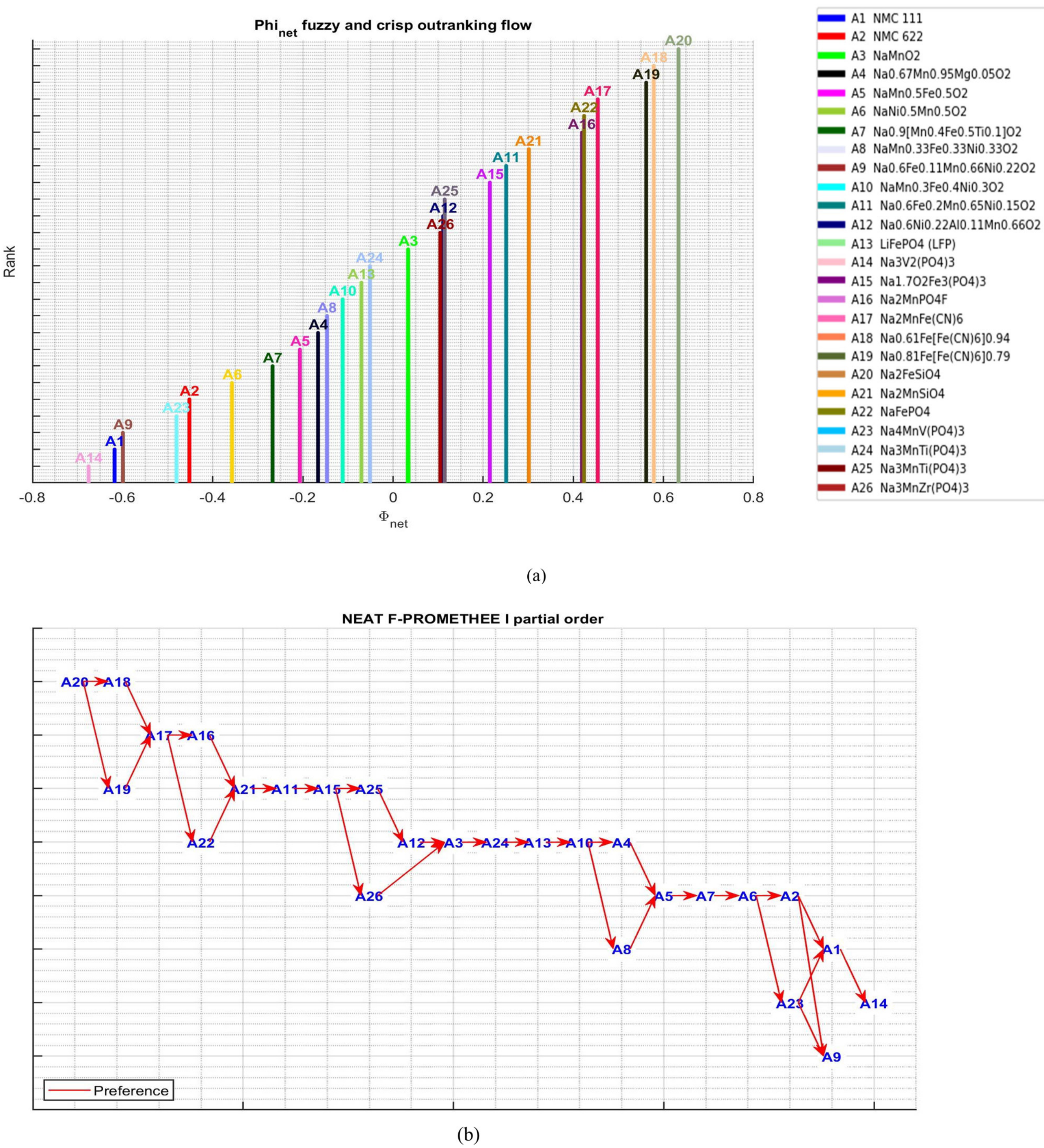


Fig. 12 Ranking of alternatives with cost of CAM in 2035: (a) net ranking and (b) partial order ranking.

$(CN)_6]_{0.94}$ † and Na_2FeSiO_4. If energy density is varied (*x*-axis), impacts may change significantly. Here, the energy density is varied in % and the real numbers are provided for the corresponding CAM. Also, it has to be noted that a full cell may have a different energy density, as indicated by the theoretical energy density values for metallic anodes (Li– for LIBs and Na for SIBs) or state of the art materials such as graphite (for LIBs) and hard carbon (for SIBs). Still, these values are theoretical and are further minimized by *e.g.* the selected electrolyte and separator.[5]

Besides the variation of energy density, which is difficult to be set as there are several parameters affecting it, other factors also matter. This has been shown for the cost, taking current values and projected values for 2032. Also, SR can change over time and the selected region. Taking for example, the supply risk indications from the EU, which is updated every three years, changes

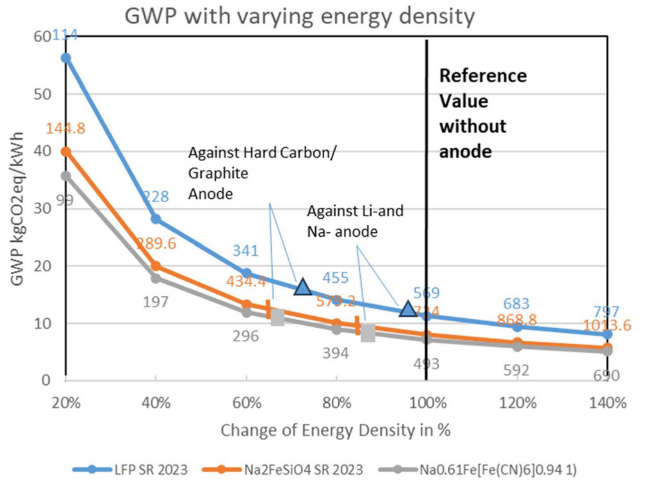


Fig. 13 Sensitivity analysis for GWP and three selected CAMs with varying energy densities. The reference energy density is highlighted by the bold line and contrasted to theoretical energy density values against metallic Li/Na anodes and state of the art hard carbon and graphite anodes.

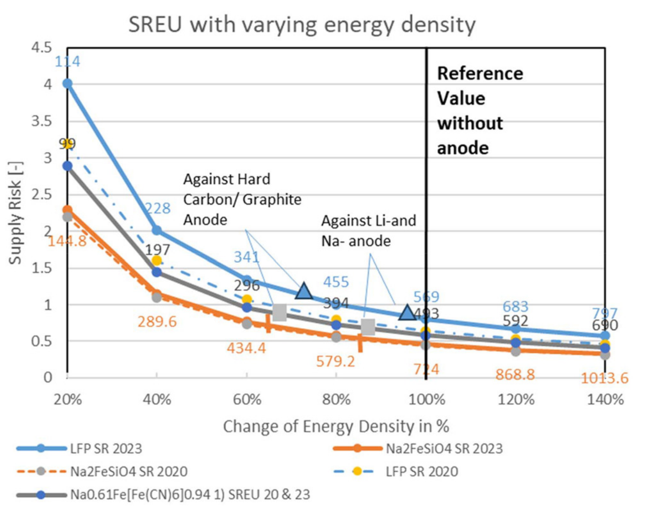


Fig. 14 Sensitivity analysis for supply risk and three selected CAMs with varying energy densities. The reference energy density is highlighted by the bold line and contrasted to different supply risks reported for the required CAM raw materials.

can be observed as indicated in Fig. 14. Again, the sensitivity against the energy density is shown for the supply risk values from 2023 and contrasted to the supply risk values from 2020 (dashed lines). It can be seen that for LFP the risk has increased as the lithium has received a higher supply risk value.

7. Limitations

The presented approach allows one to consider multiple sustainability aspects at once and entails a comprehensive sensitivity analysis. However, there are several limitations related to the work. First, all considered technologies have different TRLs, making comparison difficult. This is especially so for the low TRL of some selected SIB chemistries where only scarce or no data exists. Most of the limitations are described in detail in the cited papers on SIB sustainability[5] and toxicity screening;[12] thus only major aspects are highlighted here. Also, there are other interesting indicators that could be included, if available, in screening, *e.g.* reliability, various additional performance indicators (thermal performance, charging tolerance, safety)[76] or potential implications of concrete mining activities in specific countries in social terms (child work, working accidents).[77]

Furthermore, all values used for the CAMs are based on theoretical values derived from laboratory-scale assessment often related only to the component or half-cell and are related to high uncertainties. However, these theoretical values allow different CAMs to be comparable. The values reflect the properties of the CAM and not a full cell, which can lead to a very different picture as indicated in the sensitivity analysis. Such differences become obvious in the comparison of full SIB and LIB cells, as in Peters *et al.*, where SIBs do not perform better on a cell level. There is also a big difference in the current technical performance of full cells, where SIBs show lower performance regarding *e.g.* specific energy and cyclability.[78,79]

Additionally, recycling is not considered, which can lead to a shift in results. Taking closed loop recycling for LiNCM can have a high impact and might not be economically feasible for some SIB-based chemistries using abundant materials such as iron cyanide or manganese.[25] Very limited studies discuss the strategies for recycling sodium batteries.[80,81] To date, there are no established recycling processes for selected SIB CAMs, making it difficult to take this phase into account.

Beyond this, some data on the SR of critical raw materials may change over time as shown in the sensitivity analysis. For example, the SR of lithium may change significantly if supply becomes more diversified, or if European refinement capacities are increased. Here, the values used reflect only a snapshot in time. The same is true for the used cost, which has been modelled *via* Monte Carlo simulation until 2035. However, the price developments over the past 5 years have shown that it is barely possible to make robust price predictions due to the influence of unpredictable market dynamics.

The CO_2 footprint of the precursors is based on only one scenario for energy supply and mining (see the SI for details). Consequently, selecting a certain provider for a precursor can lead to different results. A good example is the provision of vanadium pentoxide, which was modelled on conversion routes in South Africa, which is rather CO_2 intensive.[82] Other routes could be production *via* steel or oil production. The same is true for the results of the toxicity screening which is based on available 'hazard classification' data provided by the European Chemical Agency (ECHA). The used values for THP calculation include non-harmonised data with a notification threshold of 50, which is a rather conservative approach.[12] However, some CAMs can be labelled as potentially hazardous if this threshold is lowered to 0, as in the case of Prussian blue chemistries. This stems from the fact that there is no experience with some of the materials used in new CAMs. As for the other indicators, values thus might change over time and lead to a new picture.

The method applied does not reflect the weights of real stakeholders but is based on the fulfilment of the consistency index of comparisons carried out with the AHP. Involving stakeholders in the process for preference elicitation can have an impact on the results. While HFL-TOPSIS is sensitive to the choice of normalisation, NEAT-Fuzzy-PROMETHEE requires careful definition of preference functions and threshold parameters, as minor variations can substantially affect the resulting rankings. Furthermore, obstacle degree analysis, while effective in identifying critical limiting factors, does not provide a comprehensive ranking and is contingent upon the accuracy of data weighting schemes. Collectively, these limitations of the proposed method underscore the necessity for cautious interpretation of the results and the implementation of robustness assessments when comparing alternative systems.

The limitations show that there is a high need to support such screening in an iterative manner, parallel to the further developments and knowledge gain of technology developers. Adding further indicators, like social ones, could also change the results significantly and should be considered in future assessments.

8. Conclusions

The study aimed to design a comprehensive framework for evaluating the sustainability aspects of different CAMs for SIBs, also addressing uncertainty to reach a higher level of robustness for the novel approach. Due to mentioned limitations of this approach, the results should be considered as indicative in early TRL, and evaluations need to be repeated in a regular manner alongside further technology development. The screening approach incorporates multi-dimensional assessment factors like energy density, cost, GHG emissions, SR and toxicity aspects, categorised under different sustainability dimensions discussed previously. The study used an HFL-AHP method to compute the criteria weights and the NEAT-Fuzzy-PROMETHEE method to assess the rank of the CAM alternatives. A novel obstacle degree analysis was also applied to identify performance bottlenecks, while sensitivity validation improves robustness. The hybrid objective–subjective MCDM method, *i.e.*, OSWMI incorporated with CRITIC, is used to validate the criteria weights, and HFL-TOPSIS is involved to evaluate the robustness of the final outcome of the solution under different weight scenarios. This reinforces the credibility and stability of the results. Furthermore, the study also incorporates future-oriented assessments by analysing the rank variation under projected CAM costs for 2035 to acknowledge time dependence and the critical importance of long-term economic feasibility in sustainable material selection.

The assessment result shows that among the evaluation criteria, energy density, cost and GHG hold the highest weights, each exceeding 17.5%. Upon inclusion of the toxicity parameter, these top criteria maintain their prominence, while toxicity also emerges as an important factor with a notable contribution to the overall decision-making process. The decision-making evaluation indicates that alternative A20 (Na_2FeSiO_4) emerged as the highest-ranked alternative with a net crisp value of 0.573 when toxicity is not included. Due to its high energy density, low-cost and abundant material compositions, it emerges as an optimal solution. When input-related toxicity is considered, $Na_{0.61}Fe[Fe(CN)_6]_{0.94}$ † (A18) secured the highest position with a net crisp value of 0.4948, benefiting from its significantly lower non-toxic profile (of precursors for manufacturing) and environmental compatibility. However, this is based on a harmonized hazard statement for CN-based precursors and could be different in practice. Widely used CAMS like NMC 111 and NMC 622, for comparison, are lower ranked due to their high cost, SR and potential higher toxicity. Although current LFP cells exhibit higher technical performance compared to polyanionic SIBs, their overall ranking is weakened by the increasing supply risk of Li from 2023, and the criticality of phosphate. Since the assessment is carried out with the NEAT-Fuzzy-PROMETHEE method, the result depends on the function which is considered as U-shaped in this analysis. As a result, the performance gap is reduced between LIBs and SIBs, and LIBs frequently occupy an intermediate position in the ranking. The applied sensitivity analyses enhance the robustness of the proposed framework by clarifying both the structural drivers of performance and the influence of key factors on the ranking of CAMs. The obstacle degree analysis identifies toxicity and energy density as the dominant barriers across alternatives, providing insight into the main factors limiting sustainability performance. Complementary sensitivity evaluations show that ranking outcomes can change when critical parameters are varied. The results are particularly sensitive to the assumed energy density, temporal and regional changes in cost, GWP and supply risk data. However, the rankings may vary as technical, economic and supply-chain conditions evolve; the proposed methodology is intended to be generic and novel. Additionally, the presented approach can be used as a blueprint for the screening of future emerging CAM chemistries at early TRL, or even if at higher TRL, the real-world data available extended on the cell level considering technical performance and further sustainability aspects from a life cycle perspective. This offers a flexible and reliable tool to support and guide research in next-generation battery materials.

Author contributions

Dr Sayan Das: conceptualization; methodology; formal analysis and investigation; writing – original draft preparation and review and editing. Dr Manuel Baumann: conceptualization; data curation; writing – original draft preparation; and review and editing. Dr Marcel Weil: conceptualization; funding acquisition; resources; supervision; and review and editing.

Conflicts of interest

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

Abbreviations

AHP	Analytic hierarchy process
CAM	Cathode active material
CI	Consistency index
CR	Consistency ratio
EOL-RIR	End of life-recycling input rate
FLTS	Fuzzy linguistic term set
GHG	Greenhouse gas
HES	Hybrid energy system
HFL	Hesitant fuzzy logic
HFLTS	Hesitant fuzzy logic term set
LIB	Lithium-ion battery
$LiFePO_4$	Lithium iron phosphate battery
MCDM	Multi-criteria decision making
NEAT-Fuzzy-PROMETHEE	New easy approach to preference ranking organization method for enrichment of evaluations
NIS	Negative ideal solution
OWA	Ordered weightage average
PBA	Prussian blue analogue
PIB	Potassium-ion battery
PIS	Positive ideal solution
RCI	Relative closeness index
RI	Random index
SSbD	Safe and sustainable by design
SDGs	Sustainable development goals
SIB	Sodium-ion battery
SR	Supply risk
TRL	Technology readiness level
TFN	Triangular fuzzy number
THP	Total hazard point
TrFN	Trapezoidal fuzzy number
TOPSIS	Technique for order of preference by similarity to ideal solution
VIKOR	VlseKriterijumska optimizacija i kompromisno resenje

Symbols

$\check{c}_i$	Matrix
env (H_s)	HFLTS envelope
P	Subset within the range of
G_h	Grammar used in the linguistic term set (LTS) S
H_s	Subset of S
$h_p(y)$	Function
$\check{r}_i$	Row number
S	$\{s_o, \ldots, s_g\}$ is the set of linguistic terms
S_{ll}	Domain of the expressions generated by G_h
Y	Set

Data availability

The authors declare that all the datasets are publicly available.

Supplementary information (SI) is available. See DOI: https://doi.org/10.1039/d6gc00637j.

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