

REVIEW

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# A systematic review on life cycle assessment (LCA) of metal-organic frameworks (MOFs) and MXenes

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## Abstract

Life Cycle Assessment (LCA) is increasingly recognized as an effective tool for evaluating the environmental sustainability of emerging chemicals. While metal-organic frameworks (MOFs) and MXenes show exceptional functional properties for applications such as carbon capture, catalysis, and energy storage, their environmental impacts remain underexplored and fragmented across the literature. Given the rapid expansion of research into MOFs and MXenes, and the growing emphasis on sustainability in materials science, this review is both timely and necessary to consolidate existing LCA efforts and guide future assessments toward more holistic and standardized approaches. This systematic review examines 26 papers applying LCA to MOFs and MXenes, highlighting environmental hotspots, methodological limitations, and trade-offs between functional performance and sustainability. For MOFs, solvent use and energy-intensive synthesis dominate environmental burdens, while the impacts of MXenes—particularly  $Ti_3C_2T_x$ —are chiefly tied to the high electricity demand and hazardous etchants. Most studies adopt cradle-to-gate boundaries and rely on lab-scale data, limiting their relevance for industrial-scale deployment. Additionally, current MXene LCAs focus narrowly on Ti-based systems, overlooking the broader material family. This review underscores the need for standardized LCA approaches, integration of toxicity and functional performance metrics, expanded coverage of life cycle stages and synthesis routes to support the sustainable development of these advanced materials. Future research should expand life cycle coverage, integrate toxicity and performance metrics, and address methodological gaps to better align environmental assessments with material innovation.

**Keywords** Environmental sustainability, Metal-organic framework, MXene, Green chemistry, Sustainable chemistry, PRISMA

## 1 Introduction

Life Cycle Assessment (LCA) has become an increasingly important methodology for evaluating the environmental impacts of products, processes, and services throughout their entire life span—from raw materials extraction to end-of-life (EoL) disposal [1–3].



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Its ability to capture the full spectrum of environmental impacts across a product's life cycle makes LCA an essential tool for identifying hotspots, guiding process improvement, and supporting science-based sustainability decisions in both industry and policy.

LCA's credibility is reinforced by internationally recognized standards such as ISO 14,040 [4] and ISO 14,044 [5]. Global initiatives, including sector-specific guidelines from the World Business Council for Sustainable Development (WBCSD) [6] and harmonization efforts by the European Commission [7], further support its application. The growing integration of LCA into policy frameworks—such as the European Union (EU) Renewable Energy Directive—and its expanding presence in scientific literature [8] demonstrate its increasing importance in the implementation of sustainable industrial practices.

In the chemical industry, where intensive resource use and emissions are persistent concerns, LCA supports informed and responsible decision-making by quantifying environmental impacts and identifying opportunities for process optimization [9, 10]. LCA is a core component of the Safe and Sustainable by Design (SSbD) framework [11], especially for chemicals, nanomaterials, and advanced materials. As a pre-market approach, SSbD integrates safety and sustainability from the design phase to avoid unintended trade-offs and support a toxic-free, climate-neutral future [12].

Unlike traditional efficiency metrics like eco-balance or atom economy, LCA extends its scope to endpoint-level assessments, capturing broader environmental damage including human health risks, resource depletion, and ecosystem quality. When combined with complementary approaches such as exergy and thermodynamic analysis, and supported by process simulation tools (e.g., Aspen Plus, CHEMCAD) [13], LCA enables a comprehensive and physically grounded evaluation tool for chemical processes, particularly in early-stage or data-scarce scenarios.

A major challenge in applying LCA to chemical processes—especially at industrial or pilot scale—is the limited availability of detailed data [14], often due to confidentiality constraints. This is a serious hindrance, because the accuracy of LCA results depends heavily on the availability of high-quality Life Cycle Inventory (LCI) [8] data, which involves detailed accounting of all material and energy inputs, outputs, emissions, and waste within well-defined system boundaries. As a result, practitioners frequently settle for scaled-up laboratory data, which, if not handled carefully, can introduce significant uncertainty. Additionally, energy requirements for the process are often omitted due to their sensitive nature, further compromising data completeness [15].

The LCA methodology addresses these challenges by offering structured guidance for managing data gaps, ensuring that critical aspects such as energy use, mass balance, and product system completeness are not overlooked. For novel substances with limited experimental data, initiatives like CheMatSustain promote the use of in-silico quantitative structure-activity relationship models (QSARs), in vitro methods, and New Approach Methodologies (NAMs) to generate essential data for both risk assessment and LCA [11, 16].

Metal-organic frameworks (MOFs) and MXenes provide meaningful examples of the importance of conducting an early-stage assessment of the environmental implications of emerging chemical products.

The 2025 Nobel Prize in Chemistry is awarded to Susumu Kitagawa, Richard Robson, and Omar M. Yaghi for the development of MOFs, highlighting their transformative

impact on materials science and applications [17]. The first reported examples of MOFs in 1995 featured crystalline, thermally stable, microporous frameworks with zeolite-like architectures, such as a cobalt-carboxylate network (Co-BTC) with  $7 \times 10 \text{ \AA}$  channels and selective aromatic guest binding, and a copper-bipyridyl framework with large rectangular channels (up to  $43 \times 18 \text{ \AA}$ ), both demonstrating remarkable stability and porosity [18, 19].

The MOFs are a class of porous crystalline materials formed by coordinating metal ions or clusters with organic ligands [20]. MOFs possess unique structural, physical, and chemical properties, including controllable porous structures, tuneable composition, and excellent thermal and chemical stability, making them promising for diverse applications [21] such as gas storage and separation, catalysis, wastewater treatment, particularly in adsorption of heavy metals and organic pollutants, biomedical applications, and in energy conversion devices like supercapacitors, batteries, and fuel cells. Recent advancements have focused on developing more sustainable and energy efficient synthesis methods for MOFs, involving bio-organic ligands, greener solvents, reduced reaction times, lower solvent volumes, and solvent recycling strategies to address issues like toxicity, and instability associated with conventional approaches [22]. However, challenges persist in scaling up MOF production due to high cost of raw materials, and the extensive use of solvents, especially N, N-dimethylformamide (DMF).

First discovered in 2011, MXenes are a rapidly expanding family of two-dimensional (2D) transition metal carbides and nitrides, featuring exceptional electrical conductivity, mechanical strength, and a large specific surface area [23]. While over 50 different compositions of MXenes have been produced [24] and dozens more have been theorised computationally, over 70% of research has focused so far on the initially discovered  $\text{Ti}_3\text{C}_2\text{T}_x$  [25]. MXenes are being explored for various applications, including energy storage in batteries and supercapacitors, electromagnetic interference (EMI) shielding, and catalysis [26]. Yet, their broader adoption is hampered by high production costs, susceptibility to oxidation, and the reliance on hazardous etching methods like hydrofluoric acid (HF) [27]. There is a recognized priority in the development of safer and more eco-friendly synthesis methods, including fluorine-free etching and bottom-up approaches [28].

Although MOFs and MXenes are widely studied for their exceptional functional properties, systematic evaluations of their environmental sustainability remain scarce and fragmented. Existing LCA efforts are limited in number, vary in scope, and often differ in system boundaries, modelling depth and approaches, making cross-comparison difficult. This gap is critical because early-stage sustainability assessments can guide material design and scale-up toward safer and more sustainable pathways. A comprehensive review is therefore timely to consolidate current knowledge, identify methodological shortcomings, and outline clear directions for future research.

The development of advanced materials like MOFs and MXenes, while technologically promising, requires critical evaluation of their environmental sustainability to facilitate their transition from lab-scale to industrial deployment. To address this, we systematically reviewed 26 LCA studies of MOFs and MXenes, following the PRISMA (Preferred Reporting Items for Systematic reviews and Meta-Analyses) [29] methodology. This approach provides structured guidance for transparent, complete, and accurate reporting of systematic reviews, aiming to ensure the trustworthiness and replicability of

findings. Ultimately, the analysis of the literature about the LCA of MOFs and MXenes highlights the urgent need for robust environmental assessments to guide the sustainable design and production of these emerging materials.

## 2 Research methodology

### 2.1 Questions formulation

This review aims to answer the following research question: How has LCA been applied to evaluate the environmental impacts of MOFs and MXenes, selected as model emerging chemicals, and what are the critical gaps, methodological limitations, and environmental hotspots identified in the current body of literature?

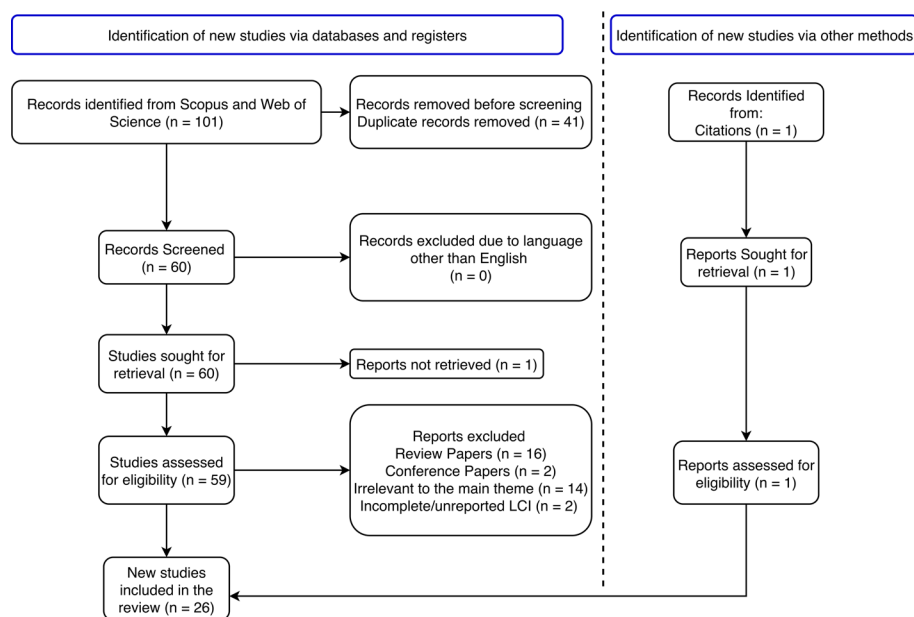
### 2.2 Locating studies

This study employs a systematic literature review (SLR) methodology, conducted in accordance with the PRISMA guidelines [29]. The objective was to identify and analyse peer-reviewed studies that explore the application of LCA in the context of MOFs and MXenes.

The literature search was carried out using two databases: Scopus and Web of Science. The search strategy was constructed using Boolean operators and parenthesis to combine the keywords: ["Life Cycle Assessment" OR "Life-Cycle Assessment" OR "LCA"] AND ["MOF" OR "MXene"]. This initial query yielded a total of 101 records.

The screening process was conducted in three sequential stages as highlighted in Fig. 1. In the first stage, duplicate entries were identified and removed, resulting in 60 unique records. Language was also considered as a screening criterion. However, no studies were excluded on this basis, as all identified articles were published in English.

The second stage involved verifying the availability of records; one study was excluded due to inaccessibility, as the full text was not available through institutional or open-access channels, leaving 59 studies for further evaluation.



**Fig. 1** PRISMA diagram [29] adapted for the current study

The third stage focused on assessing the eligibility of the remaining studies based on predefined inclusion and exclusion methodological criteria. Studies were excluded if they were review articles that did not place LCA at the core of their analysis ( $n=16$ ), conference proceedings ( $n=2$ ), or if they were deemed irrelevant to the central theme of the review ( $n=14$ ). Additionally, studies that failed to provide a complete or clearly defined LCI were also excluded ( $n=2$ ). To ensure comprehensiveness, one additional study was identified and included through citation tracking.

Following this rigorous selection process, a total of 26 studies were deemed eligible and included in the final review, as detailed in Table S1. These studies form the basis for the subsequent analysis and synthesis of findings regarding the integration of LCA methodologies in the development and application of MOFs and MXenes.

Although only 11 studies explicitly state adherence to ISO standards, all follow practices consistent with ISO 14,040 [4] and ISO 14,044 [5] standards. Among the 26 studies, 3 explicitly used an attributional LCA approach and 1 adopted a consequential approach, while the rest did not specify the modelling framework.

When assessing the environmental performance of emerging materials such as MOFs and MXenes, it is essential to differentiate between attributional (ALCA) and consequential (CLCA) LCA, as they pursue fundamentally different conceptual objectives. ALCA is a descriptive, accounting-based approach that provides a “snapshot” of the share of global environmental burdens attributable to a given product within its existing life cycle. In contrast, CLCA is decision-oriented and examines the environmental consequences—direct and indirect—arising from a specific change, such as an increase in demand for a novel material [30].

These methodological differences become particularly evident in the treatment of multifunctionality and system boundaries [31]. ALCA typically applies partitioning or allocation procedures, distributing impacts among co-products according to physical or economic relationships in order to preserve additivity—that is, ensuring that individual product LCAs collectively sum to total global impacts. CLCA, on the other hand, avoids allocation by employing system expansion and substitution, modelling marginal production and market-mediated effects to capture how the wider economic system responds to a decision. While ALCA is often guided by deontological, responsibility-based ethics focused on past and present impacts, CLCA is grounded in consequential ethics, making it more suitable for supporting prospective, decision-relevant sustainability evaluations [31].

Importantly, because these two approaches differ in goal, system modelling, boundary definition, and handling of multifunctionality, their numerical results are not directly comparable. Even when applied to the same material system, ALCA and CLCA quantify fundamentally different types of environmental burdens—average versus marginal—and therefore may lead to divergent conclusions. As a result, cross-study comparisons must carefully account for the underlying methodological framing to avoid misleading interpretations.

### 3 Results

#### 3.1 Goal and scope definition and system boundaries

The definition of goal and scope in LCA varies considerably across the reviewed studies, reflecting differences in data availability, technological maturity, and the intended

application of the materials. While many studies indicate the potential uses of MOFs or MXenes—such as for carbon capture and storage (CCS), hydrogen separation, nitrogen fixation, or electrocatalysis—the majority limit their LCA scope to the production or synthesis phase, commonly referred to as “cradle-to-gate”. This approach excludes downstream processes such as material use, regeneration, and EoL treatment, often due to the early-stage development of these technologies and the lack of reliable data.

Of the 26 studies analysed, 18 were performed at the laboratory scale, while only 8 incorporated assessments of scaled-up production settings, often using established methodologies such as the framework proposed by Piccinno et al. [14] to estimate environmental impacts at industrial scale. However, scaling up from lab-scale data introduces additional layers of uncertainty, particularly when assumptions about process efficiency, energy consumption, and material recovery are not yet validated at industrial level.

For instance, Dutta et al. [32] and Grande et al. [33] noted that the absence of large-scale applications and unknown material lifespans precluded a sound cradle-to-grave analysis. Similarly, Hansen et al. [34] and Jia et al. [35] excluded use and EoL phases due to uncertainty in future applications and insufficient data. Other studies, such as those by Mohamed and Bicer [36], Ntouros et al. [37], and Pioquinto-García et al. [38], focused on laboratory-scale synthesis, within the cradle-to-gate boundaries.

Only a small subset of studies extended their scope beyond production to include material use, regeneration, and EoL processes. Notably, Hu et al. [39] integrate MOF regeneration and metal recycling into a broader CCS system analysis. Tao and Brander [40] conducted a cradle-to-grave consequential LCA, incorporating manufacturing, utilization, and recycling of degraded MOFs. Wang et al. [41] similarly included adsorbent regeneration and solvent recovery in their system boundaries.

In the case of MXene-related LCA studies, the definition of goal and scope is generally characterized by narrow system boundaries, with most assessments only focusing on the synthesis phase. This cradle-to-gate approach dominates the literature, reflecting both the early stage of MXene commercialization and the limited availability of data on downstream processes.

The primary objective across these studies was to quantify the environmental impacts associated with MXene synthesis, often at the laboratory scale. For instance, Dadashi Firouzjaei et al. [42] assessed the cumulative energy demand (CED) [43] and environmental burdens of  $Ti_3C_2T_x$  production, while Ungureanu et al. [44] conducted a comparative LCA of seven different synthetic pathways for the same MXene. These studies also aimed to identify environmental hotspots and explore optimization opportunities for greener synthesis options, comparing MXenes with conventional materials (e.g., copper or aluminium foils) or evaluating different synthesis routes for the same MXene type.

Although the use phase and EoL were typically excluded, a few studies contextualized their assessments within specific applications. For example, Carvalho et al. [45] evaluated sodium-ion batteries using MXene anodes, while Srivastava et al. [46] and Zu et al. [47] examined MXene-based electrocatalysts and Fenton-like systems, respectively. However, even in these cases, the downstream impacts were either qualitatively discussed or completely omitted due to data limitations. System boundaries consistently included raw material extraction, MAX phase synthesis, etching and delamination processes, energy and solvent consumption, and in some cases, waste treatment.

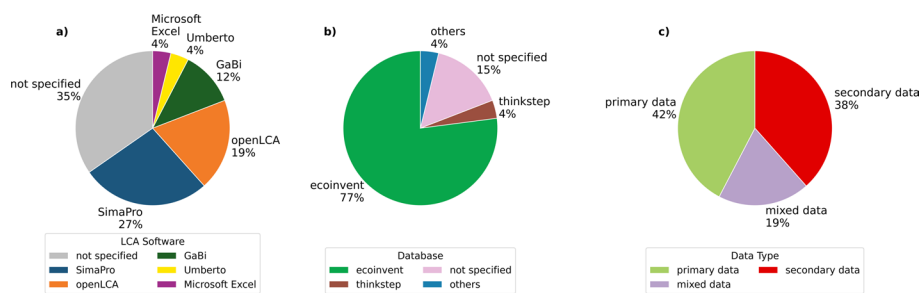
Most studies acknowledged the lack of reliable data on material degradation and EoL treatment as a major limitation to conducting full cradle-to-grave assessments. Nonetheless, some studies, such as Zu et al. [48], addressed catalyst cycling and material longevity, suggesting that extending the lifespan of MXenes could significantly reduce environmental impacts.

Functional units varied depending on the study's focus, ranging from mass-based units (e.g., 1 kg of dry MXene) to application-specific metrics (e.g., 1 kWh of battery capacity or 1  $\mu\text{mol}$  of contaminant removed).

### 3.2 Life cycle inventory

The scrutiny of the selected studies reveals notable variation in the LCA modelling tools employed, as detailed in Table S2. While some studies clearly specify the software used to construct and analyse the LCI, a significant portion (35%, 9 studies) do not disclose the software used (Fig. 2a). Among those that do, SimaPro [49] is the most frequently used, appearing in 27% of the studies (7 studies), followed by openLCA [50] in 19% (5 studies). Other tools include GaBi [51] (11%, 3 studies), Umberto [52] (4%, 1 study), and Microsoft Excel (4%, 1 study). Beyond usage frequency, the choice of LCA software can affect results. For instance, comparative studies showed that SimaPro and GaBi often yielded similar outcomes, but differences in database structures and impact assessment methods could lead to significant discrepancies, sometimes altering conclusions. This uncertainty is not captured by Monte Carlo simulations, underscoring the need for transparency in reporting software and database versions and for harmonization through standardized validation protocols such as ring tests [53].

In terms of LCI databases, the analysis of the literature revealed a strong preference for ecoinvent [54], which was employed in 77% of the studies analysed (20 out of 26), as observed in Fig. 2b. This widespread use suggests ecoinvent's role as the most common reference for environmental data in LCI modelling of emerging materials such as MOFs and MXenes. In contrast, only one study (4%) utilized the thinkstep [55] database, and another referenced alternative sources for inventory modelling (e.g., Nuss and Eckelman [56]). Notably, 4 studies (15%) did not specify the database used, raising concerns regarding transparency and reproducibility. The lack of consistent reporting on database selection may limit comparability across studies, since background data significantly influence impact outcomes. Limited coverage of datasets for specialty in databases often forces practitioners to approximate with similar substances or omit flows, which can significantly affect impact results and increase uncertainty.

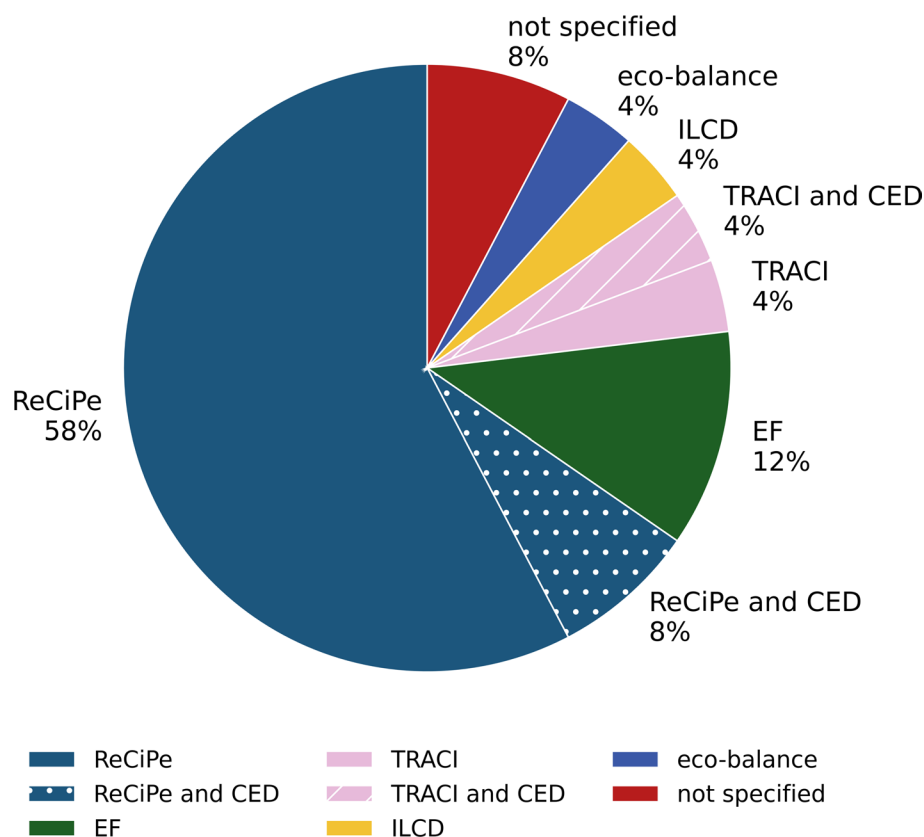


**Fig. 2** Overview of key characteristics across the reviewed LCA studies: (a) LCA software used; (b) LCI databases employed; (c) Data quality classification (primary, secondary, mixed)

In terms of data quality, 42% of the studies (11 out of 26) relied mainly on primary data, oftentimes obtained from laboratory experiments. A mixed data approach was adopted in 5 studies (19%), where either primary data were scaled up to industrial levels using scale-up frameworks [14], or the inventories were supplemented with data from the literature (see Fig. 2c). However, 10 studies (39%) reported the use of secondary data for the LCI, obtained from the literature. Both primary and secondary data modeling inherently involve further calculations and assumptions, particularly for estimating atmospheric emissions. It is essential to explicitly state where direct measurements were used and where assumptions begin—detailing the applied equations, scale-up frameworks, simulations, or mathematical models.

### 3.3 Life cycle impact assessment

The selection of the impact assessment method across the reviewed studies shows a clear preference for a few widely recognized frameworks, though some variability remains, as noted in Fig. 3 and Table S2. ReCiPe [57] was the most frequently applied method, used in 17 out of 26 studies (65%). The Environmental Footprint (EF) method [58] was applied in three studies (11%), while TRACI [59] was used in two studies (8%). The ILCD [60] and eco-balance methods were each used in 1 study (4%). CED [43] was not used alone, but appeared in three studies (12%) as an additional indicator for different types of energy use—two times alongside ReCiPe and one with TRACI. Notably, two studies (8%) did not specify the impact assessment method employed.

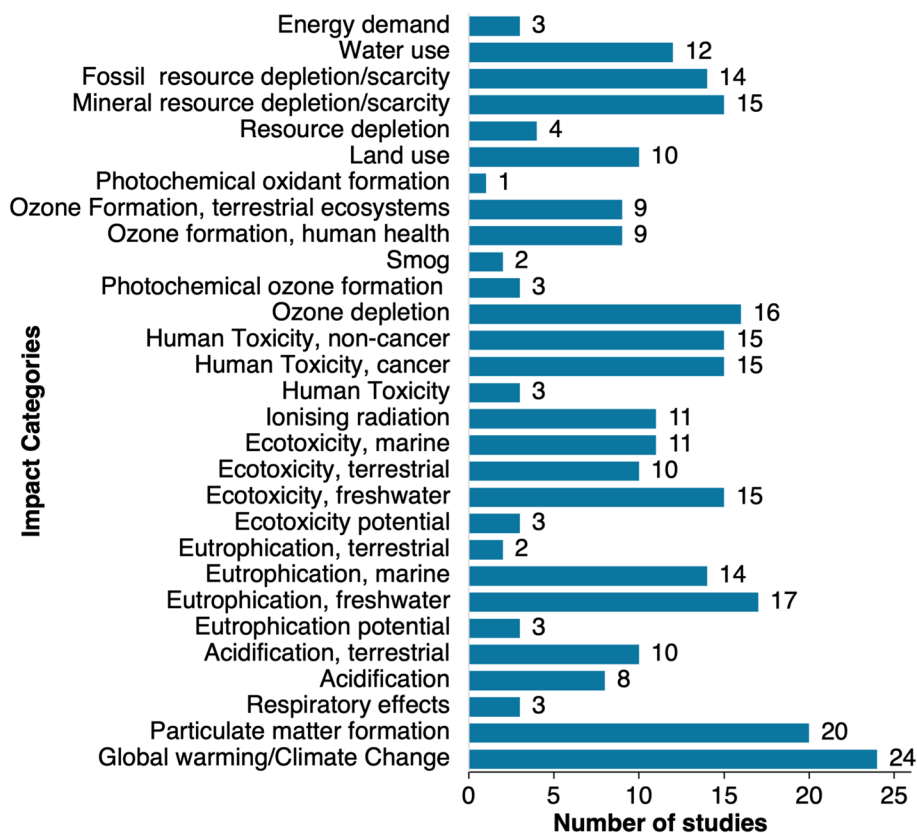


**Fig. 3** Overview of the applied LCIA methods across the reviewed studies

Although only a few impact assessment methods have been applied in the research papers analysed, they are inherently different, and this poses a challenge for cross-study comparisons. Each method defines its own set of impact categories, and while some categories may overlap conceptually, they often differ in terms of coverage, characterization models, and units used to express the results. These methodological differences can lead to variations in how environmental impacts are quantified and interpreted, limiting the comparability of findings across studies.

Regarding the level of detail in impact category reporting, most studies focused exclusively on midpoint indicators ( $n = 21$ ), while 1 study used only endpoint indicators, and 4 studies reported both. 11 studies reported between 16 and 18 impact categories, while 4 studies reported 10–15 categories, 8 studies focused on 2–9 categories, and 3 studies addressed a single issue, such as climate change.

As illustrated in Fig. 4, climate change emerged as the most frequently addressed impact category assessed in 24 studies, which demonstrates its central role in environmental impact analysis, due to national and international policies and frameworks driving towards carbon neutrality in the near future. Close behind, respiratory effects and particulate matter formation were considered in 23 studies, reflecting growing concern about the direct and indirect emissions of fine particulate associated with chemical processes. Other frequently evaluated categories included freshwater eutrophication (17 studies), ozone depletion (16 studies), and three equally represented indicators—human toxicity (cancer and non-cancer), freshwater ecotoxicity, and mineral resource



**Fig. 4** The impact categories across the reviewed studies

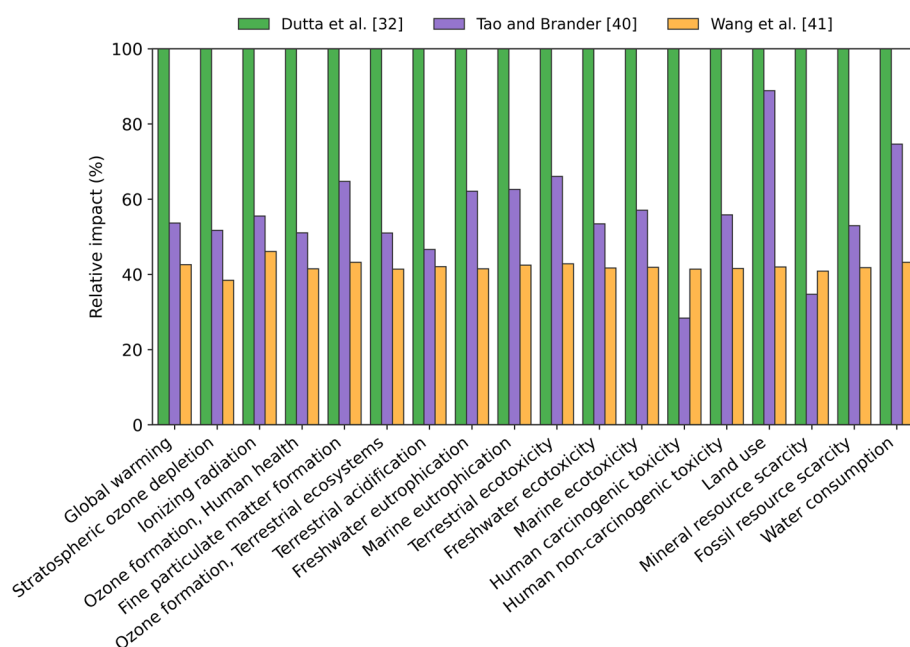
scarcity—each appearing in 15 studies. Marine eutrophication and fossil resource depletion followed closely, each addressed in 14 studies.

### 3.4 Cross-comparison of LCA results across studies

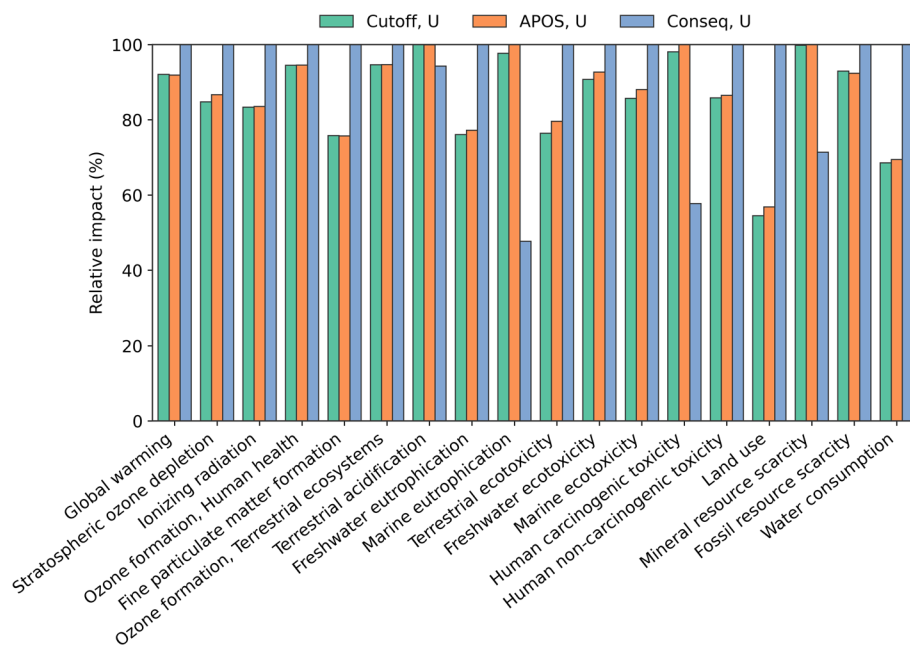
MOF-74-Mg has been assessed in several studies included in this review [32, 39–41, 61, 62]. Ideally, for cross-comparison purposes, both the underlying inventory datasets and the absolute impacts obtained from the LCA should be reported. Since most studies only provide relative or normalized results, and just a few include the associated foreground inventories, we conducted a harmonized comparison using the available data. To this aim, the inventories described in each study were imported into SimaPro and evaluated using the same database, modelling approach and impact assessment method indicated in the original studies. This approach ensured comparability of results under consistent methodological conditions.

The outcomes, presented in Fig. 5, reveal notable variability across studies. The highest impacts are associated with the inventory from Dutta et al. [32], whose system boundaries include additional purification and activation steps that substantially increase solvent consumption—particularly DMF—resulting in impacts up to 74% higher than those obtained from the other inventories. By contrast, Tao and Brander [40] and Wang et al. [41] report broadly similar starting inventories, yet their outputs still differ across categories. These deviations are significant, for some indicators up to 46% (land use), reflecting the influence of the modelling approach (attributional vs. consequential) even when the input data are comparable.

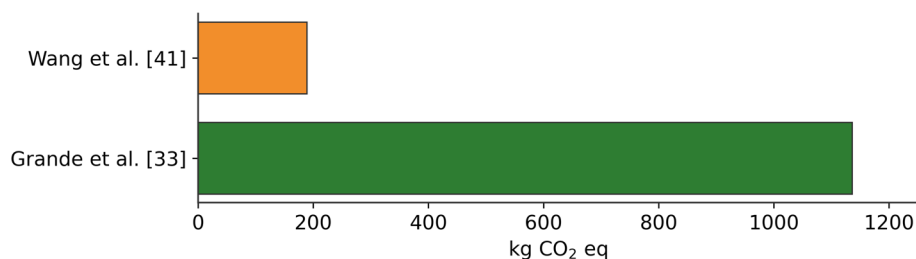
To directly assess the effect of the LCA modelling approach, the two attributional models (APOS, U and Cutoff, U) were compared with the consequential model (Conseq, U) using the inventory published by Tao and Brander [40]. Differences between the two attributional approaches remain small, with variations of up to 3% per category, as



**Fig. 5** Comparative analysis of relative impacts for the production of 1 kg of MOF-74-Mg across three literature sources (Dutta et al. [32]; Tao and Brander [40]; Wang et al. [41]). Results are harmonized using the ReCiPe 2016 Midpoint (H) method applied to the inventories reported in the corresponding studies



**Fig. 6** Comparison of Cutoff, U; APOS, U; and Conseq, U system models for 1 kg of MOF-74-Mg, based on the inventory of Tao and Brander and evaluated with ReCiPe 2016 (H)



**Fig. 7** Global warming impact for 1 kg of MOF-74-Ni according to Grande et al. [33] and Wang et al. [41], calculated using the ILCD 2011 Midpoint method

indicated in Fig. 6. In contrast, the consequential model introduces more pronounced changes, particularly for marine eutrophication (52%), human carcinogenic toxicity (43%), and land use (43%), illustrating the sensitivity of certain impact categories to the underlying modelling framework.

A further comparison was performed for MOF-74-Ni using the data from Grande et al. [33] and Wang et al. [41]. Although both studies consider similar synthesis routes, their respective scale-up frameworks differ considerably, resulting in distinct solvent consumption and energy requirements at industrial scale. The inventory constructed by Wang et al. [41], based on their specific scale-up assumptions, reflects lower solvent use and improved energy efficiency, which in turn leads to an 83.2% lower climate change impact compared with the value reported by Grande et al. [33], as shown in Fig. 7. It should be noted that [33] provided only the absolute impact for global warming; therefore, this comparison is limited to that category. For [41], impacts were derived from their published inventory using the same procedure applied to the other studies and analysed with the ILCD 2011 Midpoint method to ensure consistency with the assessment of the first study.

In the context of the LCA of  $Ti_3C_2T_x$  MXene, a comparison between the impacts reported by Ungureanu et al. [44] and those published earlier by Dadashi Firouzjaei et al. [42] (Fig. 8a)—both evaluated using the TRACI 2.1 method—shows markedly higher values in the former, with differences ranging from 72% to 83% across the assessed categories. This substantial increase mainly reflects the additional contributions included in the more recent assessment by Ungureanu et al. [44], such as precursor production, process energy, and atmospheric emissions, which were only partially accounted for in the study by Dadashi Firouzjaei et al. [42].

A second cross-comparison was performed for an alternative synthetic pathway using results from Ungureanu et al. [44] and Hansen et al. [34], with the former recalculated under EF 3.1 to ensure methodological consistency with the latter (Fig. 8b). Since Hansen et al. [34] reported only six impact categories, the comparison is necessarily restricted to these indicators. Importantly, Hansen et al. [34] employed an industrial-scale modelling approach, whereas the model developed by Ungureanu et al. [44] is based on laboratory-scale inventories. The impacts calculated from the model developed by Ungureanu et al. [44] are over 95% higher for all impact categories, underscoring the influence of scale-up assumptions and the uncertainties related to inventory completeness in MXene production studies.

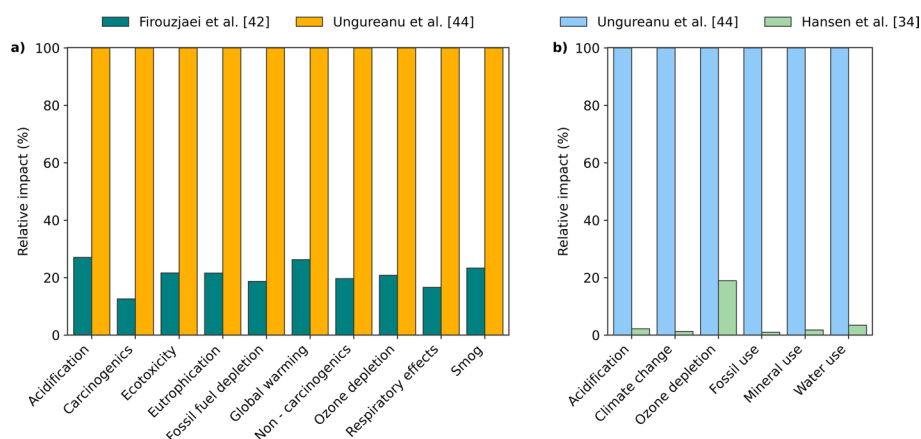
## 4 Discussion

### 4.1 Main factors contributing to the environmental impacts of MOFs

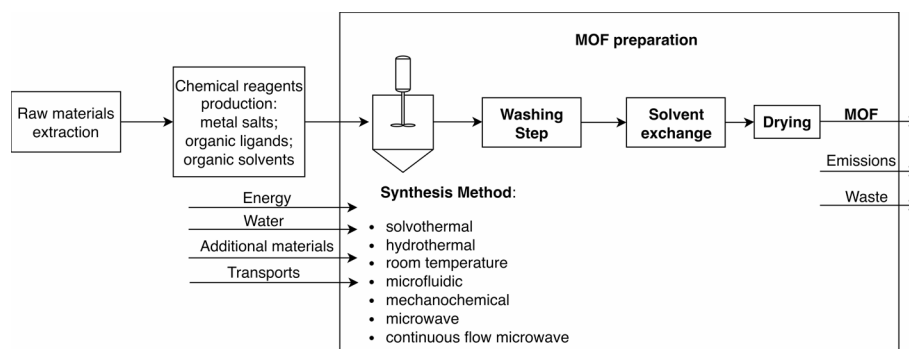
A general flowchart illustrating the production of MOFs is presented in Fig. 9. The process begins with the extraction of raw materials, followed by the production of chemical reagents such as metal salts, organic ligands, and solvents.

The synthesis methods evaluated in the reviewed studies include solvothermal, hydrothermal, room temperature (RT), microfluidic, mechanochemical, microwave-assisted (MW), continuous flow microwave and reactive extrusion techniques.

After synthesis, MOFs typically undergo a series of activation steps, beginning with extensive washing using large volumes of solvent to remove unreacted precursors and byproducts—necessary for maximizing surface area and porosity. In some cases, a solvent exchange step is introduced, replacing the synthesis solvent with one of lower



**Fig. 8** Relative environmental impacts associated with the production of 1 kg of  $Ti_3C_2T_x$  MXene: **(a)** comparison between Firouzjaei et al. [42] and Ungureanu et al. [44], evaluated using the TRACI 2.1 LCIA method; **(b)** comparison between Ungureanu et al. [44] and Hansen et al. [34], with the former recalculated under EF 3.1 for methodological consistency



**Fig. 9** General flowchart for the production of MOFs

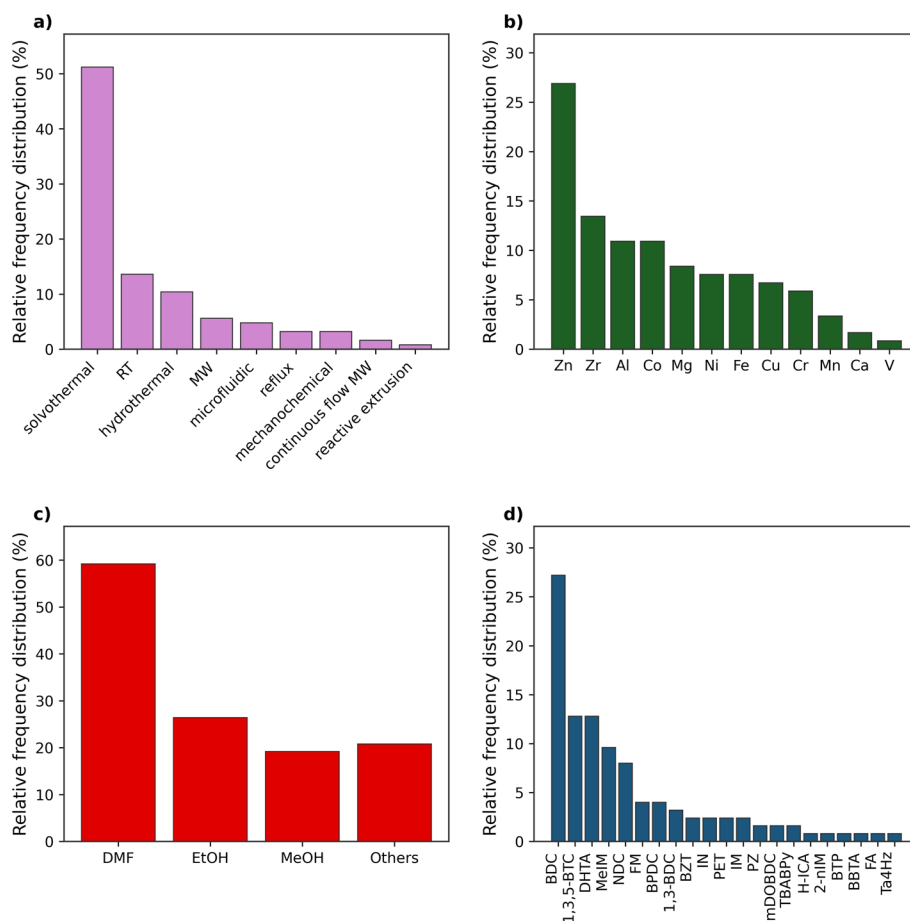
surface tension and boiling point to prevent pore collapse [63]. The final stage is drying, which can be carried out under vacuum or at atmospheric pressure, ensuring complete removal of residual solvents from the porous structure.

The examination of the 19 studies focused on the LCA of MOFs identified a total of 125 distinct case studies, as detailed in Table S3. The most frequently investigated MOFs included ZIF-8, MOF-74-M (where M = Co, Mg, Ni, Zn), MIL-101(Cr), and MIL-53(Al).

A wide range of synthesis methods was employed across these studies, with the most frequently assessed being solvothermal (51%), room temperature (14%), and hydrothermal (10%) (see Fig. 10a). The choice of the synthesis method (e.g., solvothermal, microwave, reactive extrusion, mechanochemical, hydrothermal) and the subsequent purification stages show significant contributions to the environmental footprint of MOFs. Dutta et al. [32] found that microwave synthesis exhibited lower environmental impacts compared to other methods, such as solvothermal synthesis, largely due to its significantly reduced solvent requirements. Escobar-Hernandez et al. [64] demonstrated that reactive extrusion for ZIF-67 production largely reduced environmental and health impacts (by approximately 3–5 orders of magnitude) with respect to the traditional solvothermal technique. Chang et al. [65] introduced a method for directly synthesising MIL-100(Fe) from iron ore concentrates, which reduced synthesis cost by half and enhanced environmental sustainability compared to conventional methods using elemental iron or iron salts. Yang et al. [66] also proposed an eco-friendly synthetic pathway for V-MOFs starting from waste gasification, aiming to reduce the harmful emissions associated with conventional methods.

In terms of chemical composition, the most commonly used metal ions were zinc (27%), zirconium (13%), aluminium (11%), cobalt (11%), magnesium (8%), nickel (8%), and iron (8%) (see Fig. 10b).

Solvents play a central role throughout the synthesis, washing, activation, and solvent exchange steps, with *N,N*-dimethylformamide (DMF) being the most popular (59%), followed by ethanol (26%) and methanol (19%) (see Fig. 10c). A variety of other solvents—accounting collectively for 21% of the studies—were also reported, including *N,N*-dimethylacetamide (DMA), *N,N*-diethylformamide (DEF), dimethylsulfoxide (DMSO), acetonitrile, dichloromethane (DCM), triethylamine (TEA), acetone, isopropanol, *N*-methyl-2-pyrrolidone (NMP), chloroform, and ionic liquids such as 1-ethyl-3-methyl-imidazolium bromide ([EMI]Br) and 1-Methyl-3-octyl-imidazolium-bromide (OmimBr).



**Fig. 10** Relative frequency distribution across the reviewed LCA studies of MOFs in function of: (a) synthetic method employed; (b) metal ion employed; (c) organic solvent used; (d) organic linker used

The nature and quantity of solvents are repeatedly identified as the most significant contributors to the environmental footprint of MOFs. Organic solvents, such as DMF and NMP, often lead to high environmental impacts. For instance, DMF is frequently cited as a major hotspot due to its substantial contribution to categories like climate change, human toxicity, fossil depletion, and particulate matter formation. Rico-Barragan et al. [67] found that using DMF added notable environmental impacts on MIL-101(Cr) synthesis, with its production being the hotspot for human toxicity due to barium leaching into water. Ntouros et al. [37] highlighted that DMF and methanol accounted for more than 85% of the overall environmental impacts in synthetic routes where they were used as both solvents and washing agents. Additionally, Grande et al. [33] demonstrated that the utilisation of solvents for cleaning and purification can have an equal or even larger impact on some environmental indicators than the synthesis of MOFs itself. Pioquinto-García et al. [38] found that using DME, dichloromethane (DCM), and hexane for solvent exchange step significantly increased environmental damage in DUT-4 synthesis, compared to solvothermal synthesis without solvent exchange. Conversely, studies by Grande et al. [33], Pioquinto-García et al. [38] and Dutta et al. [32] showed that using water as a solvent can significantly reduce environmental impacts, sometimes by several orders of magnitude for CO<sub>2</sub> emissions, freshwater toxicity, and resource depletion. Furthermore, the lack of effective solvent recycling practices increases the environmental

burdens of MOF syntheses. De Miranda et al. [68] proved that incorporating aluminium recovery and reducing the volume of solvent used in MIL-53(Al) synthesis led to significant reductions in environmental impacts across multiple categories.

The most widespread organic linkers included benzene-1,3-dicarboxylic acid (1,3-BDC, 27%), 1,3,5-benzenetricarboxylic acid (1,3,5-BTC, 13%), 2,5-dihydroxyterephthalic acid (DHTA, 13%), 2-methylimidazole (MeIM, 10%) and 2,6-naphthalenedicarboxylic acid (NDC, 8%) (see Fig. 10d).

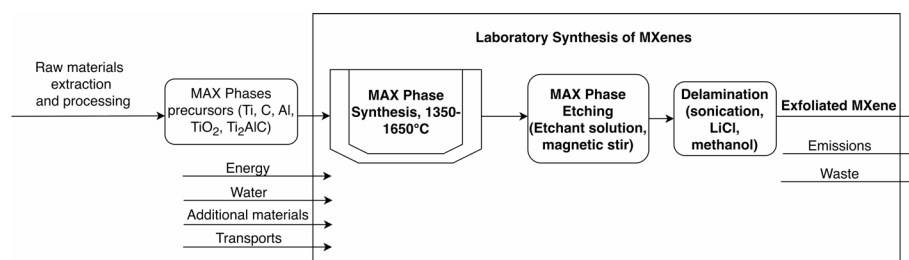
The energy required for MOF synthesis and activation, typically in the form of electricity and heat, is another substantial contributor to environmental impacts. The impact is particularly pronounced when energy is sourced from fossil-fuel-dependent grids. For example, Ntouros et al. [37] found that electricity consumption, especially due to Greece's fossil-fuel-dependent energy mix, accounted for up to 13% of the overall environmental impacts in some ZIF-8 synthetic routes. The calcination of MOFs or their precursors at high temperatures, as mentioned by Wu et al. [69] for biochar-based MOFs, also employs significant amounts of energy. Even low-energy methods, such as room-temperature synthesis, can still result in high overall footprints if they necessitate large amounts of environmentally harmful solvents or extensive washing steps.

The production of precursors, including metal salts and organic ligands, also contributes to environmental burdens, although often to a lesser extent than solvents. However, in some cases, their impact can be substantial. Escobar-Hernandez et al. [64] noted that the production of metal salts (nitrates) for ZIF-67 synthesis requires significant volumes of nitric acid, which is derived from ammonia. Ultimately, this leads to a noticeable environmental contribution due to the fossil fuels used in ammonia production. Rico-Barragan et al. [67] identified that chromium (III) nitrate nonahydrate production directly contributes to metal depletion in MIL-101(Cr) synthesis.

#### 4.2 Main factors contributing to the environmental impacts of MXenes

Recent LCA studies on MXenes—particularly  $Ti_3C_2T_x$ —have highlighted the main environmental impacts associated with their production, as highlighted in Table S4. Within the cradle-to-gate boundaries, the assessment typically comprises raw material extraction, processing and transports, MAX phases synthesis (where MAX phases are layered carbides and nitrides serving as the precursors of MXenes), MAX phases etching and subsequent delamination, to yield the corresponding exfoliated MXene (see Fig. 11). The LCA may also take into consideration the energy use for additional processes, such as metal powders production, waste treatment, equipment manufacturing.

The main environmental burdens associated with MXenes stem from three interrelated factors: high energy consumption throughout the synthesis and delamination



**Fig. 11** General flowchart for the production of MXenes

workflow, the employment of various toxic reagents such as hydrofluoric acid, and the production of MAX phases.

Electricity consumption has emerged as a dominant environmental hotspot in the laboratory-scale synthesis of  $Ti_3C_2T_x$  MXenes, with multiple studies consistently reporting that it accounts for the majority of the total environmental burden. For instance, Dada-shi Firouzjaei et al. [42] found that electricity use contributes over 90% of the environmental impacts for gram-scale production and around 70% for kilogram-scale batches, primarily due to energy-intensive steps such as high-temperature MAX phase synthesis, multiple cycles of centrifugation and thermal control during etching and delamination. Zu et al. [47] reported that electricity consumption accounted for 76% of the CED and 52.7% of the total environmental damage in MXene/Fe/PMS systems.

Additionally, in the production of a  $NiMoSe/Ti_3C_2T_x@CC$  electrocatalyst [46], electricity was the primary driver of multiple impact categories, including acidification potential, global warming potential, human toxicity, particulate matter, fossil resource use, and water use.

The high energy demand of MXenes is largely due to the MAX phase synthesis, which typically involves heating to 1400 °C for 1–2 h, accounting for 57% of the total electricity consumption [42].

The energy mix used for electricity generation plays a pivotal role in determining the overall environmental footprint of MXenes. Systems reliant on fossil fuels—such as hard coal in China or India—exhibit significantly high impacts [47]. In contrast, shifting to renewable energy sources, such as the present-day electricity mix in Sweden, or future decarbonized grids, can drastically reduce environmental burdens of MXenes. For instance, using 100% renewable electricity for  $Ti_3C_2T_x$  synthesis has been shown to reduce CED by 52% and GWP by approximately 70% compared to fossil-based scenarios [42]. Zu et al. [47] found that MXene/Fe/PMS system exhibited 54% renewable energy, when powered by Swedish electricity.

Among chemical precursors, titanium powder is a major environmental hotspot, contributing over 70% of the chemical-related impacts due to the energy-intensive Kroll process used in its production [34]. Lithium chloride (LiCl), often used in delamination, significantly contributes to mineral resource scarcity and accounts for about 10% of overall chemical impacts.

MXene synthesis frequently involves hazardous etchants such as hydrofluoric acid (HF) and hydrochloric acid (HCl), which pose risks to both human health and the environment. HF emissions, in particular, contribute to terrestrial acidification [44]. While alternative organic etchants—such as dimethyl sulfoxide (DMSO), urea, tetrabutylammonium hydroxide (TBAOH), choline hydroxide, and n-butylamine—are being explored, they also present hazards due to flammability or corrosivity [34].

The synthesis process generates waste containing acid and metal traces, including residues of Ti and Al, as well as solid particulates. However, the environmental contribution of these waste flows is generally minor compared to electricity and chemical inputs. Nevertheless, metal sludge recycling has been proposed as a strategy to reduce environmental damage from landfilling and to enable the regeneration of precursor materials [47].

The environmental impacts of  $Ti_3C_2T_x$  MXene synthesis are highly dependent on the specific synthetic route employed. Key determinants include reaction time, temperature,

chemical inputs, laboratory equipment, and production yield, all of which influence energy consumption and material efficiency. Among the various strategies assessed [44], the original HF-based method demonstrated the lowest environmental impacts across most categories, primarily due to its short reaction time and room-temperature etching, which significantly reduce electricity demand. Alternative approaches, such as LiF-HCl etching, exhibit higher environmental impacts—approximately 3.7 times greater in end-point single-score assessments—due to extended reaction durations.

Greener approaches such as the waste tire-derived carbon-based MAX phase synthesis show promise in reducing environmental burdens, particularly during MAX phase production. By incorporating secondary aluminium, titanium dioxide, and tire-derived carbon, this method can reduce environmental impacts by up to 30% when used as a precursor in subsequent MXene synthesis routes [44].

#### 4.3 Trade-offs between environmental impacts and functional performance

MOFs have emerged as highly promising materials across carbon capture, adsorption, catalysis, and energy applications, offering exceptional functional performance due to their tuneable porosity, high specific surface area, and chemical versatility. In CCS applications, several MOFs outperform conventional MEA scrubbing in terms of energy efficiency and CO<sub>2</sub> capture [39, 41]. However, their environmental impacts—especially from synthesis solvents like DMF—can offset these performance gains. For example, while Zn-MOF-74 shows lower environmental impacts than its Mg counterpart, MEA still exhibits lower total environmental impacts [40].

Beyond CO<sub>2</sub> capture, MOFs like MIL-100(Fe), MIL-101(Cr), and DUT-4 demonstrate high adsorption capacities for dyes, VOCs, and siloxanes, often surpassing activated carbon [38, 65, 67]. MOF-biochar composites further enhance mechanical strength and environmental performance, offering a more sustainable alternative to traditional adsorbents [69, 70]. In catalysis and energy storage, MOFs such as MIL-101(Fe) and MIL-88 A(Fe) exhibit high efficiency in ammonia production [36] and pollutant degradation, while MOF-based cathodes in zinc-ion batteries exhibit a high rate performance [66].

Although many studies compare the environmental impacts of different MOF synthesis scenarios, trade-offs with functional performance are rarely examined. When alternative synthetic strategies are considered, a lower environmental impact may coincide with reduced material performance. For example, hydrothermal synthesis of DUT-4 showed lower environmental impacts than solvothermal routes but resulted in a lower siloxane adsorption capacity, making the solvothermal option more favourable when considering both impact and functionality [38]. In contrast, some trade-offs were synergistic: using iron ore for MIL-100 (Fe) instead of iron salts improved adsorption capacity while reducing impacts across most categories [65]. Other cases showed marginal trade-offs, such as MIL-53 (Al) production with reduced reaction time and solvent recovery, which slightly improved environmental burden and adsorption capacity, though differences were small [68]. In such cases, Monte Carlo uncertainty analysis should be applied to validate whether observed improvements are statistically significant.

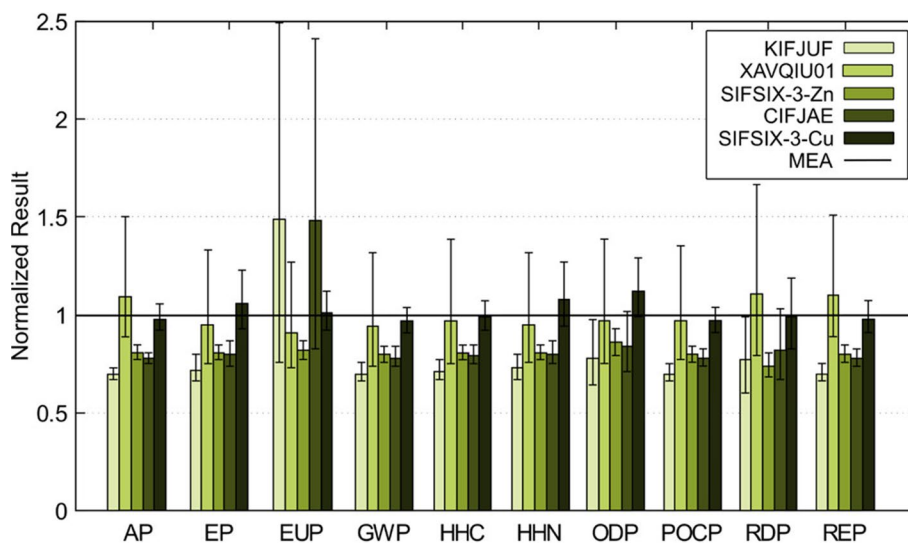
In a recent study, Hu et al. [39] evaluated the environmental performance of several top-performing MOFs for post-combustion CO<sub>2</sub> capture by normalizing their life-cycle impacts to MEA, the conventional benchmark for CCS. Their ranking also accounted for the estimated electricity requirement for CO<sub>2</sub> separation and compression, derived from

an energy-consumption model optimized individually for each structure. As illustrated in the reproduced figure Fig. 12 [39], the analysis reveals distinct trade-offs: SIFSIX-3-Zn achieves the lowest average impacts, around 20% lower than MEA; CIFJAE and KIFJUF offer 19–32% reductions in most categories but show elevated eutrophication impacts due to the use of dimethylacetamide (DMA); and XAVQIU01 presents lower eutrophication burdens than MEA but higher impacts in acidification, resource depletion, and respiratory effects. Under optimized synthesis conditions, the minimum-impact results indicate that CIFJAE and KIFJUF can reduce their eutrophication burdens by up to ~20%, making all three MOFs environmentally competitive with—or even outperforming—SIFSIX-3-Zn under best-case assumptions. This highlights the strong sensitivity of MOF rankings to process-level assumptions and the importance of considering synthesis-related uncertainties in comparative assessments.

Given the versatility of MOFs, trade-off considerations should extend beyond conventional gas storage and separation to encompass advanced applications that leverage their high porosity, large surface area, and structural and chemical tunability. This multifunctionality positions MOFs as promising components in technologies such as heterogeneous catalysis (e.g., electrocatalytic reactions), magnetic MOFs (MMOFs), (LEDs), and nanomedical platforms for high-capacity drug delivery and biosensing [21].

Similar considerations apply to MXenes, where outstanding functional properties introduce new challenges for sustainable design.

MXenes are distinguished by their high electrical conductivity, a defining property that places them among the most advanced materials in electronics. Remarkably, MXenes exhibit the highest conductivity of all synthetic 2D materials, surpassing reduced graphene oxide (rGO) films by more than an order of magnitude [71]. For instance, optimised synthesis of  $Ti_3C_2T_x$  MXene can produce materials with conductivities of approximately 15,000 S/cm, comparable to conventional metals [72]. Beyond conductivity, MXenes offer tuneable surface chemistry, flexibility, transparency, and solution processability, making them highly suitable for applications such as EMI shielding and flexible electrodes [73]. However, their electronic properties are highly sensitive



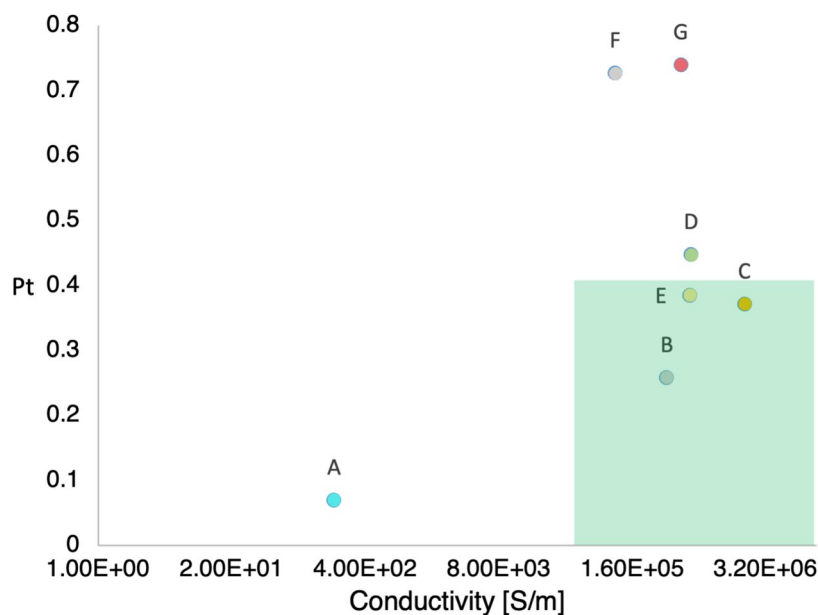
**Fig. 12** Environmental impact trade-offs for five top-performing MOFs for CO<sub>2</sub> capture. Results are normalized to MEA and presented from left to right according to the MOFs' estimated energy requirement for CO<sub>2</sub> separation and compression. Error bars indicate the minimum and maximum normalized impacts.

to synthesis conditions, surface terminations ( $-T_x$ ), and defect density, requiring precise control to achieve optimal material properties.

Recent LCA studies integrated performance metrics into environmental assessments, enabling a more holistic evaluation of synthesis strategies. Notably, trade-offs have been identified between environmental impacts and electrical conductivity in  $Ti_3C_2T_x$  MXene synthesis. While certain synthesis pathways exhibit lower environmental profiles, others deliver superior electrical conductivity, emphasizing the importance of balancing sustainable design with performance metrics.

Building on this perspective, Ungureanu et al. [44] explored how environmental burdens relate to electrical performance by jointly plotting the single-score impact (Pt) against the bulk electrical conductivity of various  $Ti_3C_2T_x$  MXene synthetic routes. When represented in this way (Fig. 13, adapted from [44]), a distinct high-desirability region emerges—corresponding to low environmental impacts combined with high conductivity—within which three pathways (B, C, and E) consistently fall. Although the precise density of  $Ti_3C_2T_x$  films may vary across reported values, ranging typically from 2 to  $4\text{ g cm}^{-3}$ , the positioning of these pathways is only minimally affected by such assumptions. Overall, the analysis indicates that one pathway (i.e., B) provides the most balanced compromise when environmental performance is prioritized, whereas pathway C represents the preferred trade-off when electrical conductivity is favoured, as it delivers the highest conductivity among the assessed routes while keeping its environmental burdens within the same moderate range as B and E. These results highlight the need to balance sustainability and functional performance in MXene synthesis.

Compared to conventional EMI-shielding materials such as aluminium and copper foils, laboratory-scale syntheses of  $Ti_3C_2T_x$  MXenes exhibit markedly higher environmental impacts, primarily due to the energy-intensive nature of precursor synthesis, selective etching, and delamination. A more quantitative comparison, developed by Dadashi Firouzjaei et al. [42], shows that  $Ti_3C_2T_x$  has higher burdens than both



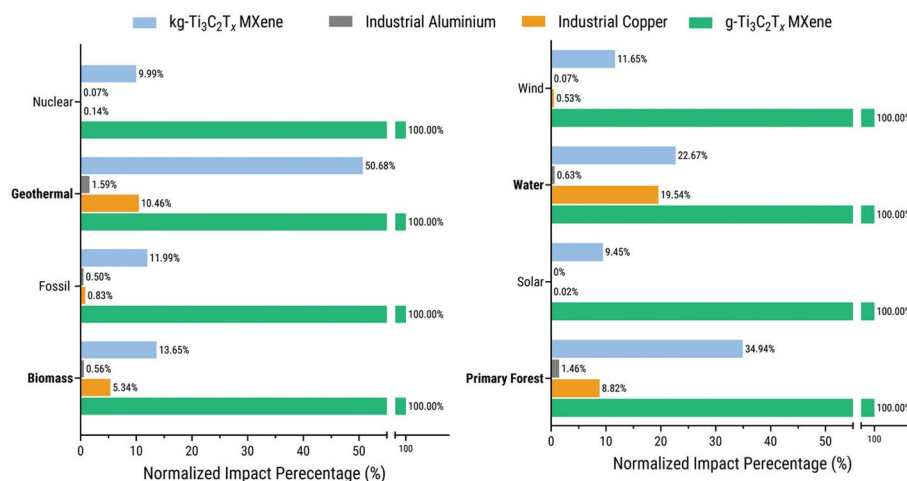
**Fig. 13** Impact–performance trade-off map for  $Ti_3C_2T_x$  MXene synthesis pathways, plotting endpoint single-score environmental impacts (Pt) against bulk electrical conductivity. The shaded region indicates the area of highest desirability (low impact, high conductivity).

metals across most categories, consistent with its substantially greater cumulative energy demand (see Fig. 14). In eight impact categories, gram-scale batches ( $\text{g-Ti}_3\text{C}_2\text{T}_x$ ) display the highest impacts, whereas scaling to kg-scale batches ( $\text{kg-Ti}_3\text{C}_2\text{T}_x$ ) reduces impacts by roughly an order of magnitude. Sensitivity analyses further indicate that MAX-phase furnace time has a measurable influence: both systems show approximately 10% lower impacts when the furnace duration is reduced from 2 h to 1 h, and around 20% higher impacts when extended from 2 h to 4 h. Overall, these results illustrate clear impact trade-offs for MXene production, highlighting the strong dependence of environmental performance on synthesis scale and thermal-processing conditions.

Beyond electronic properties, MXenes exhibit exceptional mechanical and optical characteristics that remain largely overlooked in LCA, despite their relevance to performance–environmental impacts trade-offs. For instance, their high stiffness—predicted Young’s moduli of 500–800 GPa and experimental values around 330 GPa for monolayer  $\text{Ti}_3\text{C}_2\text{T}_x$  [74] enables superior wear life compared to conventional 2D lubricants. Similarly, optical properties such as high as 90% visible transmittance in  $\text{Ti}_3\text{C}_2\text{T}_x$  films and tuneable bandgaps (0–3 eV) [75] combined with broadband absorption and plasmonic behaviour [76] make MXenes attractive for transparent electrodes and photothermal applications. These attributes drive functional advantages but also influence synthesis complexity, material flows, and energy demand—factors that shape environmental profiles. Future LCA studies should explicitly integrate mechanical and optical properties into trade-off analyses to ensure sustainability decisions reflect both functional benefits and environmental impacts, establishing robust guidelines for sustainable material design.

#### 4.4 Gaps in current LCA studies, key observations and future research recommendations

LCA is a fundamental tool for evaluating the environmental sustainability of advanced materials, yet its application to MOFs and MXenes is methodologically constrained. For MOFs, existing studies are increasing in number but often lack depth, while



**Fig. 14** Normalized environmental impacts for the production of  $\text{g-Ti}_3\text{C}_2\text{T}_x$ ,  $\text{kg-Ti}_3\text{C}_2\text{T}_x$ , aluminium foil, and copper foil, reproduced without changes from Firouzjaei et al. [42] under the CC BY-NC 4.0 license. Results were normalized to  $\text{g-Ti}_3\text{C}_2\text{T}_x$  and presented to illustrate impact trade-offs across materials and scales. Error bars indicate minimum and maximum values across the evaluated impact categories

MXene-related LCAs are still in their infancy, with only a handful of publications, as detailed in Fig. 15.

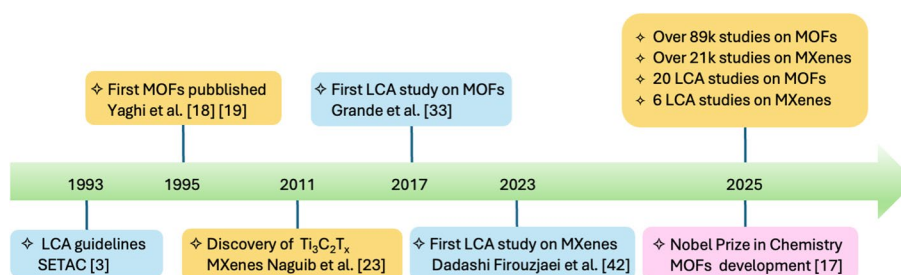
A major limitation is the narrow focus on a few impact categories—namely climate change, particulate matter, eutrophication, and human toxicity (see Sect. 3.3)—while neglecting the complete set of indicators provided by the impact assessment method. This selective reporting risks burden-shifting and obscures whether proposed pathways are genuinely more sustainable.

For instance, CCS studies frequently show reductions in climate change impacts, but increases in acidification, toxicity or resource depletion [77, 78], illustrating how category prioritization can bias technology comparisons.

Another critical gap is the cradle-to-gate focus, which excludes downstream stages such as use phase, regeneration, and EoL treatment. Emissions from MOFs degradation during the use phase and EoL scenarios such as recycling or disposal are rarely considered. This omission limits the ability to identify potential environmental trade-offs in applications involving regeneration cycles and hazardous degradation products.

While incineration and landfill disposal are the primary EoL scenarios for spent MOFs, these traditional routes present significant environmental and technical risks, including high energy requirements, the release of stored carbon, and the ecological complexity of synthetic organic linkers [79]. To mitigate these hazards, research has increasingly focused on sustainable alternatives like regeneration, which uses activation techniques such as thermal/vacuum treatment or supercritical CO<sub>2</sub> extraction to remove guest molecules while maintaining structural integrity [80]. For example, ZIF-8 particles packaged in rigid mesoporous silica nanocapsules can successfully undergo ten in situ degradation–reconstruction cycles through vapor-assisted reconstruction [81]. Beyond simple reuse, spent MOFs are valuable progenitors for high-performance nanomaterials; specifically, the thermal transformation of MOF-199 (HKUST-1) microrods can yield monoclinic copper oxide (CuO) nanoparticles (100–250 nm) that are highly effective for room-temperature desulfurization [82]. Additionally, exhausted materials can be repurposed for secondary functions, such as converting spent gas adsorbents into efficient photocatalysts for wastewater remediation, where the presence of accumulated sulfide and sulfate species actually improves dye degradation efficiency. Emerging chemical strategies also allow for the facile digestion of rigid frameworks using bicarbonate or carbonate salts, enabling the recovery of valuable organic ligands and the extraction of embedded precious metal nanoparticles, such as palladium (Pd) nanoparticles, from a Pd@PCN-224 framework [63].

Despite the rapid expansion of MXene research, their EoL considerations and ultimate fate remain significantly less explored than their synthesis and initial applications [83].



**Fig. 15** Timeline of MOF and MXene research and LCA milestones (1993–2025)

When these materials are disposed of or released into the environment, they are highly susceptible to oxidative deterioration and hydrolysis upon exposure to air or water, which causes their layered 2D structure to break down into carbon byproducts and titanium dioxide that may negatively impact ecosystems. Persistent concerns also exist regarding their potential for long-term persistence and bioaccumulation following their eventual discharge. However, promising sustainable scenarios involve the mechanochemical regeneration of spent materials; for instance, a spent MXene-based adsorbent can be re-transformed back into the original MAX phase by milling it with aluminum powder [84]. In this recycling process, captured organic pollutants and any pillaring agents are carbonised and incorporated into the carbide structure, allowing the material to be re-synthesised for further use indefinitely. Consequently, future research must shift toward establishing standardised protocols for safe disposal and effective material recovery to mitigate these long-term environmental risks [85].

Solvent-related hotspots (e.g., DMF, DMA, and NMP) remain underexplored despite their disproportionate contribution up to 90% of total impacts [32]. Inventories often omit solvent recovery, waste treatment, and fugitive emissions, while adoption of greener alternatives is constrained by performance trade-offs. For example, for DUT-4, a lower BET surface area was observed in hydrothermal synthesis compared to solvothermal methods [38].

Ethanol, methanol, butanol, and isopropyl alcohol are frequently proposed as greener alternatives to DMF, and most reviewed studies confirm their potential benefits. However, trade-offs between environmental impacts and functional performance—such as catalytic activity and adsorption capacity—are rarely assessed. For example, Rico-Barragán et al. compared seven synthesis scenarios for MIL-101(Cr), finding that the ethanol-based route achieved the best balance between environmental impact, toluene adsorption capacity, and cost [67]. Despite progress in developing green solvents for MOF synthesis, options such as ionic liquids (evaluated in only two studies), deep eutectic solvents, Cyrene, supercritical CO<sub>2</sub> (scCO<sub>2</sub>), and bio-derived methanol remain largely unexplored [86]. Future LCAs should systematically evaluate these alternatives under scale-up conditions, as solvent choice can significantly influence both environmental outcomes and material performance. Notably, scCO<sub>2</sub> derived from feedstock CO<sub>2</sub> can function both as a reaction medium and a utilization pathway, offering a productive use phase for CO<sub>2</sub> that would otherwise require long-term storage.

An overlooked limitation in current LCA studies is the restricted library of organic ligands (see Fig. 10d). Although ligands are not the primary hotspot, they still contribute significantly to MOF environmental profile. Existing inventories are often incomplete, focused mainly on raw materials, while neglecting energy inputs, atmospheric emissions, side products, and catalysts. Future studies should systematically evaluate ligands using literature, patents, and databases, supported by simulation tools and scale-up frameworks. Well-structured and transparently reported inventories can serve as reference datasets for future MOF research, reducing the need for repeated modelling and enabling cumulative progress in sustainability assessments.

Despite its promising potential for Pb<sup>2+</sup> ion removal and Ag<sup>+</sup> recovery, only one study investigated a mix Zn-Co MOF [69]. This limited attention contrasts with the growing body of research demonstrating that multi-metal MOFs (MM-MOF) exhibit outstanding performance in various applications such as gas adsorption and separation (e.g., Cr<sup>3+</sup>/

Mg<sup>2+</sup> MIL-101, Co<sup>2+</sup>/Ni<sup>2+</sup>-MOF-74), heterogeneous catalysis (e.g., Cu<sup>2+</sup>/Co<sup>2+</sup>-MOF-74, Cd<sup>2+</sup>/Mn<sup>2+</sup> Porph@MOM-10, Zr<sup>4+</sup>/Ti<sup>4+</sup>-NDC-MOFs), photocatalysis (e.g., UiO-66 (Ce) doped with Ti<sup>4+</sup> and Zr<sup>4+</sup>), tandem reactions (e.g., non-stoichiometric InGa-PF), CO<sub>2</sub> reduction (e.g., UiO-66(Zr/Ti)-NH<sub>2</sub>), CO<sub>2</sub> adsorption (e.g., Mg<sup>2+</sup>/Ni<sup>2+</sup>-MOF-74), and iodine adsorption (Fe-Cu-BTC) [87–89]. Despite these advances, none of these materials have been evaluated through LCA, leaving a critical gap in understanding their environmental implications. Without such assessments, it is impossible to compare MM-MOFs with conventional MOFs or alternative materials.

Furthermore, MOF-based composites—including nanofiber structures and MOF–MXene hybrids—represent a major blind spot in current LCA literature. Only one study has addressed V-based MIL-47/CNT [66], despite the rapid growth of MOF–nanofiber composites with applications in catalysis, electrocatalysis, adsorption, separation, and catalytic degradation [90]. Similarly, MOF–MXene hybrids such as UiO-66-NH<sub>2</sub>/Ti<sub>3</sub>C<sub>2</sub>, which improve anti-fouling properties in PES membranes, have received minimal attention [91]. Their production introduces additional material flows and processing steps, creating performance-driven trade-offs that differ substantially from pristine MOFs [92].

A persistent limitation in current LCA literature is the treatment of scale-up. While modelling industrial-scale scenarios is valuable for anticipating future impacts, most studies report only scaled-up results, omitting laboratory-scale data. This omission introduces uncertainty because improvements attributed to scale may reflect optimistic assumptions (e.g., solvent recovery rates) rather than actual process efficiencies. To avoid speculative projections, future studies should report both laboratory-scale and scaled-up inventories and impact assessment results. This dual perspective clarifies the current state versus projected scenarios and reveals how environmental profiles evolve with scale, indicating the degree of change introduced by process scaling.

LCA studies on MXenes face even more pronounced limitations. Many omit key synthesis steps in their LCI, such as energy-intensive upstream processes like metal powders production.

Cross-study comparisons remain difficult, even for identical synthesis routes, because results diverge significantly due to differences in impact assessment methods (e.g., TRACI vs. ReCiPe) and from inconsistencies in inventory scope, including equipment manufacturing, precursor processing, and emissions modelling [44]. However, when inventories are detailed and both laboratory and scale-up procedures are transparently reported, models can be reproduced and compared more reliably, enabling meaningful benchmarking across studies.

Nearly all existing MXene LCAs focus on etching-based synthesis of Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>, reflecting the current state of experimental research, but failing to capture the rapidly expanding MXene family. Emerging compositions include Nb<sub>2</sub>CT<sub>x</sub>, and V<sub>2</sub>CT<sub>x</sub> [28], as well as double-transition metal such as Mo<sub>2</sub>TiC<sub>2</sub>T<sub>x</sub>, and high-entropy MXenes like TiVCrMoC<sub>3</sub>T<sub>x</sub> [93]. For instance, V<sub>2</sub>CT<sub>x</sub> MXene is widely explored for advanced energy storage systems, due to its structural stability, strong pseudocapacitive behaviour driven by multiple vanadium oxidation states, and ultrathin layers that minimize ion diffusion barriers [94]. A valuable research direction would be the comparison between V<sub>2</sub>CT<sub>x</sub>-based energy storage systems and conventional lithium-ion systems from an environmental perspective, given V<sub>2</sub>CT<sub>x</sub>'s high theoretical capacity of up to 940 mAh g<sup>-1</sup>. Beyond vanadium-based MXenes, several other non-Ti compositions such as include

$\text{Nb}_4\text{C}_3\text{T}_x$ ,  $\text{Sc}_2\text{CT}_x$ ,  $\text{Mo}_2\text{CT}_x$ ,  $\text{Ta}_4\text{C}_3\text{T}_x$ ,  $\text{Ti}_{1.1}\text{V}_{0.7}\text{Cr}_x\text{Nb}_{1.0}\text{Ta}_{0.6}\text{C}_3\text{T}_x$  [28, 93] remain largely unexplored in LCA studies despite growing prominence in experimental and computational research.

MXene—including  $\text{Ti}_3\text{C}_2\text{T}_x$  and emerging compositions—can be synthesised through a variety of methods alternative to etching, including molten salt synthesis, electrochemical etching, bottom-up methods such as chemical vapor deposition (CVD), plasma-enhanced pulsed-layer deposition (PE-PLD), as well as template-assisted and solid-state approaches [93]. Comparing these methods with traditional etching routes through LCA is essential to identify greener synthetic routes and potential trade-offs.

Material diversity further complicates sustainability assessments, particularly with the rise of nitride MXenes (TMNs) such as  $\text{Ti}_2\text{NT}_x$ ,  $\text{Ti}_4\text{NTi}_x$ ,  $\text{Sc}_2\text{NT}_x$ ,  $\text{V}_2\text{NT}_x$ ,  $\text{Hf}_2\text{NT}_x$ ,  $\text{Nb}_2\text{NT}_x$ . These offer functional advantages over conventional carbide MXenes such as superior electronic structures and enhanced catalytic properties, but impose new challenges [95]. The synthesis is resource intensive: M–N bonds exhibit lower cohesive energy than M–C bonds, increasing risks of instability during exfoliation, while nitride MAX phases require higher formation energy [96]. Incorporating LCAs of nitride MXenes is essential to guiding sustainable synthesis strategies for next-generation MXene materials.

A recurring limitation in LCAs of MOFs and MXenes is the omission of certain emissions or substances due to missing characterization factors in standard impact assessment methods. For example, one study modified ReCiPe 2016 to include the HF emissions in air [44], which are critical in the etching process of MXenes.

Yield data is another frequently missing parameter. Its absence introduces uncertainty, especially for low-conversion processes and hinders cross-study comparisons. Ideally, literature-based inventories should prioritize sources that report yields, and primary data should include this parameter explicitly. Where yields remain unknown, sensitivity analyses should be conducted to evaluate how variations in yield affect environmental impacts.

The lack of characterization factors for MOFs and MXenes in standard LCIA methodologies further constraints assessments, largely due to the lack of data on the materials' hazardous properties under long-term exposure. For MOFs, most toxicity studies focus on pristine materials, overlooking the transformations during use-phase, such as degradation-induced release of metal ions, the generation of reactive oxygen species (ROS), and the potential emissions of residual solvents trapped within MOF pores [97]. For MXenes, while some in vitro studies suggest low acute toxicity, there is little in vivo data regarding chronic effects, bioaccumulation, and environmental persistence [34].

The application of MOFs in biomedicine faces major challenges, primarily toxicity and biocompatibility [98]. Toxicity is largely influenced by physico-chemical factors such as chemical composition (metal ions and organic linkers), particle size, morphology, and stability. A key mechanism involves MOF degradation in biological systems, releasing metal ions or organic linkers that may accumulate and cause organ damage or immune dysregulation in vivo [99].

The most reported molecular mechanism of MOF toxicity is oxidative stress, driven by excessive ROS generation, often due to transition metal components [98]. Elevated ROS can damage mitochondrial membranes, lipids, proteins, and DNA, triggering inflammation, apoptosis, or necrosis. MOFs also induce mitochondrial dysfunction, inhibit ATP

production, and disrupt autophagy. Physical interactions, such as cell membrane damage from MOF adsorption or diffusion, further contribute to toxicity [100].

MOF toxicity varies widely with composition and structure. Copper-based HKUST-1(Cu) shows severe cytotoxicity, reducing HepG2 cell viability to 17% at 200  $\mu\text{M}$  and increasing ROS levels sixfold, causing apoptosis and mitochondrial rupture. Zebrafish embryos exposed to 1  $\mu\text{M}$  had a hatching rate of only 8.3%. Mn-MOF-74 exhibits the highest toxicity among MOF-74 variants [101]. Cobalt MOFs such as ZIF-67 trigger apoptosis in microglia and hemolysis via ROS [102], while NiCo-PYZ inhibits algal growth by 86% due to Ni/Co ion release [103]; Co-MOF-74 induces zebrafish morphological defects [101]. Even lower-toxicity MOFs like MIL-100(Fe) cause  $\sim 39\%$  cell mortality against Hep3B at an exposure of 64  $\mu\text{g}/\text{cm}^2$  [104]. Zinc-based ZIF-8 demonstrates size-dependent toxicity, with smaller particles (50 nm) showing higher cytotoxicity ( $\text{IC}_{50} = 15.6 \text{ mg/L}$ ) than larger ones (200 nm,  $\text{IC}_{50} = 19.7 \text{ mg/L}$ ) due to increased Zn accumulation and ROS [105]. Linker chemistry also matters: UiO-64(Zr) (fumaric acid) proved more toxic than UiO-66(Zr) (BDC), causing near-total amphipod mortality versus reduced mobility but survival for UiO-66 [106]. (Summary adapted from the review study [99])

Similarly, assessing MXene biosafety—stability, toxicity, and biodegradation—is critical for evaluating environmental and health impacts in LCA. MXene cytotoxicity is mainly caused by two mechanisms: (i) mechanical damage from sharp edges acting as “nanoknives,” destabilizing cell membranes, and (ii) ROS generation, leading to oxidative stress and cellular damage [107]. Toxicity depends on numerous factors such as composition and size: For example,  $\text{V}_2\text{CT}_x$  shows strong time- and dose-dependent effects, reducing cell viability to  $\sim 60\%$  at 50  $\mu\text{g}/\text{mL}$  after 24 h, and further after 48 h, due to vanadium oxidation [108]. In contrast, pristine  $\text{Ti}_3\text{C}_2\text{T}_x$  exhibits moderate cytotoxicity, with A549 cancer cells showing 20–90% viability and normal cells 70–100% at  $< 62.5 \text{ mg/L}$ , while thermally oxidized  $\text{Ti}_3\text{C}_2\text{T}_x$  is highly toxic ( $\sim 23\%$  viability at 500  $\text{mg/L}$ ) [109]. Smaller  $\text{Ti}_3\text{C}_2\text{T}_x$  nanosheets (0.09  $\mu\text{m}$ ) display enhanced antimicrobial activity, and  $\text{Ti}_3\text{C}_2$  quantum dots at 100  $\mu\text{g}/\text{mL}$  disrupt autophagy in human umbilical vein endothelial cells (HUVECs). DL- $\text{Ti}_3\text{C}_2$  nanosheets at 360  $\text{mg/L}$  for 24 h increased apoptosis in periodontal ligament cells fivefold. Conceivably, dose, and exposure time are also relevant. In vitro studies confirm dose- and time-dependent effects across cell lines. Surface modification with biopolymers (PEG, Poly-L-lysine, polyvinyl alcohol (PVA), Chitosan) improves stability and reduces toxicity [107]. In vivo studies using animal models indicate that modified MXenes at reasonable concentrations exhibit low toxicity, with no major inflammatory or organ changes. MXenes undergo biodegradation, accumulating temporarily in liver and spleen, where macrophages (Kupffer cells) and enzymes like myeloperoxidase mediate clearance. Degradation products are excreted via urine and feces. Ecotoxicological studies in freshwater systems show that MXene toxicity often results from physical effects [110]. For example,  $\text{Ti}_3\text{C}_2\text{T}_x$  agglomerates with algal cells, creating shading that limits light and nutrient availability, reducing photosynthetic pigments and increasing oxidative stress, even at low concentrations [111]. Ecotoxicity studies show  $\text{Ti}_3\text{C}_2\text{T}_x$  agglomerates with algae, reducing chlorophyll even at 0.001  $\text{mg/L}$  and inducing oxidative stress at 0.0001  $\text{mg/L}$ . Mitigation strategies, such as embedding  $\text{Ti}_3\text{C}_2$  in cellulose hydrogel, eliminate toxicity, and in vivo tests with

**Table 1** Current limitations and proposed research directions for LCA of MOFs and MXenes

Current limitation	Proposed research direction
Narrow focus on impact categories	Extend assessments beyond commonly reported indicators (climate change, particulate matter, human toxicity, eutrophication and acidification) to include broader environmental and health impacts.
Scale-up modelling gaps	Report both laboratory-scale and scaled-up inventories and impact results to clarify current state versus projected scenarios and quantify changes introduced by scaling.
Limited cradle-to-gate scope	Incorporate use-phase degradation and end-of-life disposal scenarios for both MOFs and MXenes to capture full life cycle impacts.
Cross-study comparability issues	Provide detailed inventories and transparent documentation of laboratory and scale-up procedures to enable reproducibility and meaningful benchmarking.
Missing yield data	Prioritize sources reporting yields; include yield in primary data; conduct sensitivity analyses when yields are unknown.
Absence of characterization factors for MOFs and MXene	Conduct <i>in vivo/in vitro</i> toxicology studies; evaluate emissions during use-phase, including material degradation
Lack of integration between toxicological data and LCA modelling	Develop frameworks that link experimental toxicity, biodegradation, and exposure data (e.g., <i>in vitro</i> , <i>in vivo</i> , and ecotoxicity assays) with fate and effect modelling in LCA; generate standardized datasets on degradation rates, ion release, ROS formation, and biological persistence to enable more realistic human toxicity and ecotoxicity assessments.
Energy hotspot during synthesis of MOFs and MXenes	Investigate renewable energy integration, energy-efficient processing strategies, and shorter, room temperature syntheses routes to minimize electricity demand.
Insufficient exploration of performance–environment trade-offs	Expand trade-off analysis beyond gas adsorption and separation for MOFs and beyond electronic properties for MXenes to include mechanical and optical characteristics.
Narrow scope for MOF LCAs	Expand coverage to MOF nanocomposites and multi-metal MOFs to capture additional material flows and performance-driven trade-offs.
Limited evaluation of alternative solvents for MOF synthesis (DMF hotspot)	Systematically assess ionic liquids, deep eutectic solvents, Cyrene, bio-based methanol, and $scCO_2$ under both laboratory and scale-up conditions, considering performance–impacts trade-offs.
Limited range of organic ligands in MOF LCAs	Broaden ligand coverage using literature, patents, and databases; apply simulation tools and transparent scale-up frameworks; publish reusable inventories for future studies.
Narrow scope for MXene LCAs	Extend assessments beyond Ti-based carbides to include V-, Ta-, Nb-, Zr-, Hf-based MXenes and nitride MXenes (TMNs).
Limited synthetic approaches considered for MXenes	Include LCAs for alternative synthesis routes such as molten salt synthesis, bottom-up methods, template-assisted, and solid-state approaches.
Delamination methods relying on LiCl for MXenes.	Explore alternative delamination techniques such as sonication or mechanical methods to minimize chemical use and associated hazards.
Titanium precursor hotspot (Kroll process intensity) for MXenes	Explore alternative Ti sourcing (e.g., recycled Ti, alternative precursors); study how alternative synthesis strategies beyond etching (molten salt, bottom-up, template-assisted, solid-state) influence this hotspot and integrate these comparisons into LCA frameworks.

$Nb_2C$ - polyvinylpyrrolidone (PVP) (20 mg/kg IV) report no organ damage, with clearance via liver, spleen, and excretion. (Data summarized from reference [107]).

The key findings are summarized in Table 1. In light of the limitations discussed, prospective LCA provides a suitable framework for evaluating the future sustainability of MOFs and MXenes. By enabling scenario-based modelling and drawing from diverse sources like experimental data, patents, and process simulations [112], it allows for more informed projections of environmental outcomes. Still, to make these assessments more robust, further research is needed to improve scale-up methodologies—particularly in estimating electricity demand, solvent use, and recovery efficiencies under realistic industrial conditions. Addressing these gaps is essential for guiding responsible development and integration of these materials into future technologies.

## 5 Conclusions

MOFs and MXenes are emerging materials hailed as game-changers in technologies such as carbon capture, catalysis, and energy storage. A timely evaluation of their potential environmental impacts while development is still at an early stage can help make them “safe and sustainable by design.” In this systematic review, 26 papers applying Life Cycle Assessment (LCA) to MOFs and MXenes were analysed. While LCA is increasingly applied to novel chemical systems, its use for these materials remains limited in scope and consistency. MOFs exhibit strong functional performance but their environmental burdens are dominated by toxic organic solvents and energy-intensive synthesis. MXenes, particularly  $Ti_3C_2T_x$ , offer unique properties—including high electrical conductivity, tunable electronic behaviour, and mechanical strength—yet face high impacts from electricity use, hazardous etchants, and titanium precursors.

In light of the cross-study comparisons and performance–impact relationships discussed in this review, it is evident that emerging materials such as MOFs and MXenes exhibit substantial variability in reported environmental profiles due to differences in synthesis routes, scale-up assumptions, modelling approaches, and data completeness. These discrepancies, together with the observed trade-offs between environmental impacts and functional performance, highlight the need for more harmonized inventories and consistent methodological frameworks to support robust decision-making and safe-and-sustainable-by-design development.

Most studies adopt cradle-to-gate boundaries and rely on lab-scale data, overlooking use-phase emissions, degradation, and end-of-life scenarios. For MXenes, current LCAs are narrowly focused on Ti-based systems and etching methods, neglecting the broader family of compositions and synthesis routes. Beyond these gaps, several critical limitations persist: narrow impact category coverage, lack of yield reporting, and insufficient exploration of performance–environment trade-offs. Future work should expand assessments to include toxicity, end-of-life scenarios, and alternative solvents (e.g., ionic liquids, deep eutectic solvents, Cyrene), as well as broaden material coverage to multi-metal MOFs and non-Ti MXenes. Scale-up modelling and transparent inventory reporting are essential to improve comparability and enable prospective LCA approaches that reflect future industrial conditions. Addressing these priorities will ensure that sustainability considerations keep pace with the rapid functional advancements of MOFs and MXenes.

### Abbreviations

[EMI]Br	1-ethyl-3-methyl-imidazolium bromide
1,3-BDC	benzene-1,3-dicarboxylic acid
1,3,5-BTC	1,3,5-Benzenetricarboxylic acid
2-nIM	2-nitroimidazole
AP	Acidification Potential
AOPs	Advanced oxidation processes
BBTA/H2BBTA	1 H,5 H-benzo(1,2-d:4,5-d')bistriazole
BDC	1,4-Benzenedicarboxylic acid
BPDC	Biphenyl-4,4'-dicarboxylic acid
BTC	1,3,5-Benzenetricarboxylic acid
BTP/H3BTP	1,3,5-tris(1 H-pyrazol-4-yl)benzene
BZT	Benzotriazole-5- carboxylic acid
CBZ	Carbamazepine
CC	Climate Change
CCS	Carbon capture and storage
CED	Cumulative Energy demand
DCM	Dichloromethane
DEF	N, N-diethylformamide

DHTA	2,5-Dihydroxyterephthalic acid
DMF	N, N-dimethylformamide
DMSO	dimethyl sulfoxide
DOBDC	2,5-dihydroxyterephthalic acid/2,5-dioxido-1,4-benzenedicarboxylate
ED	Energy demand
EF	Environmental Footprint
EMI	electromagnetic interference
EoL	End-of-life
ETP	Ecotoxicity potential
EUP	Eutrophication potential
FD	Fossil depletion
FE; FEP	Freshwater eutrophication
FETP	Freshwater Ecotoxicity
FM	Formic Acid
FRS	Fossil Resource Scarcity
FuA	Fumaric acid
FU	Functional unit
GWP	Global warming
H-ICA	Imidazole-2-carboxyaldehyde
HT, HTP	Human toxicity
HTC	Human toxicity, cancer
HTNC	Human toxicity, non-cancer
HUVEC	Human umbilical vein endothelial cells
IM	Imidazole
IN	Isonicotinic Acid
IR	Ionizing radiation
LCI	Life Cycle Inventory
LIB	Lithium-ion battery
Life Cycle Assessment	LCA
LEDs	Light-emitting diodes
LU	Land use
MD	Mineral resource depletion
mDOBDC	4,6-dioxido-1,3-benzenedicarboxylate
MEA	Monoethanolamine
ME, MEP	Marine Eutrophication
MeIM	2-methylimidazole
METP	Marine ecotoxicity
MOF	Metal-organic framework
MRS	Mineral resource Scarcity
MW	Microwave
NAMs	New Approach Methodologies
NDC	2,6-Naphthalenedicarboxylic acid
NMP	N-methyl-2-pyrrolidone
OD; ODP	Ozone depletion
OF-HH	Ozone formation, human health
OF-TE	Ozone formation, terrestrial ecosystems
OmimBr	1-Methyl-3-octyl-imidazolium-bromide
PET	polyethylene
PM, PMFP	Particulate Matter Formation
POF	Photochemical ozone formation
POFP	Photochemical oxidant formation
PRISMA	Preferred Reporting Items for Systematic reviews and Meta-Analyses
Pt	Single-score impact unit (Points)
PVA	Polyvinyl alcohol
PVP	polyvinylpyrrolidone
PZ	Pyrazine
QSAR	Quantitative structure-activity relationship
RD	Resource depletion
RE	Respiratory effects
ROS	Reactive oxygen species
rGO	Reduced graphene oxide
RT	Room temperature
RU-F	Resource use, fossil
RU-MM	Resource use, minerals and metals
SIB	Sodium-ion battery
SLR	Systematic literature review
SSbD	Safe and sustainable by Design
Ta4Hz	3,3',5,5'-azobenzene-tetracarboxylate
TAP	Terrestrial acidification
TBABPy	1,3,6,8-tetrakis (p-benzoic acid)pyrene
TBAOH	Tetrabutylammonium hydroxide
TEA	Triethylamine

TETP  
WBCSD  
WC

Terrestrial Ecotoxicity  
World Business Council for Sustainable Development  
Water consumption

## Supplementary Information

The online version contains supplementary material available at <https://doi.org/10.1007/s44371-026-00495-x>.

Supplementary Material 1.

### Author contributions

A.U. wrote the first draft of the main manuscript; A.U., R.R., and A.S. applied the rigorous PRISMA protocol for the preparation of this systematic review; R.R. and A.M.F. supervised the research; all authors reviewed the manuscript.

### Funding

This work did not receive any specific fundings.

### Data availability

Not applicable.

### Declarations

#### Ethics approval and consent to participate

Not applicable.

#### Consent for publication

Not applicable.

#### Competing interests

The authors declare no competing interests.

Received: 30 July 2025 / Accepted: 20 January 2026

Published online: 27 January 2026

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