Chemistry - Methods

Chemistry—Methods

Chemistry Europe
European Chemical Societies Publishing

RESEARCH ARTICLE OPEN ACCESS

Sustainable Preparation of Zeolitic Imidazolate Framework-8 in Water: From Early-Stage Life Cycle Assessment to the Industrial Scale

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Received: 29 January 2026 | **Revised:** 18 March 2026 | **Accepted:** 19 March 2026

Keywords: advanced material | LCA | MOF | solvothermal synthesis | water | ZIF-8

ABSTRACT

The solvothermal method is the most investigated for the preparation of zeolitic imidazolate framework-8 (ZIF-8), among the most investigated metal–organic frameworks, and many solvents have been tested for this purpose. The main aim of this work is to define an effective, practical, and sustainable synthesis of these materials, focusing our attention on water, the greenest solvent overall. We focus our analysis on a comparative life cycle assessment based on the ZIF-8 synthesis in water and dimethylformamide (DMF), the organic solvent of choice for ZIF-8 preparation, in order to discuss the preparation of an advanced material in terms of environmental sustainability. The current work aims to emphasize the water-based synthesis of ZIF-8 through the critical discussion of the current state-of-the-art that demonstrates its excellent performance. A comparative life cycle assessment between the traditional DMF-based synthesis and the water-based route is also proposed, whose results highlight the advantages of using water as a solvent in this reaction. This work highlights the future needs for a sustainable industrial scale-up of ZIF-8 preparation in water by discussing crucial aspects that should be taken into account by both academic researchers and industry.

1 | Introduction

1.1 | ZIF-8: A Fascinating MOF for Future Important Applications

In 2025, Susumu Kitagawa, Richard Robson and Omar Yaghi were awarded the Nobel Prize for the development of metal–organic frameworks (MOFs) [1], marking a turning point in the recognition of their relevance worldwide. MOFs are a versatile class of porous crystalline materials composed of metal ions connected by organic linkers, self-assembling into flexible and customizable supramolecular architectures [2, 3]. Due to their exceptional characteristics, several applications have highlighted their potential to address current global challenges related to energy, the environment, and sustainable materials design [4–7]. Among the MOFs, zeolitic imidazolate framework-8 (ZIF-8) has emerged as one of the most investigated materials, consisting of Zn^{2+} nodes linked by 2-methylimidazolate (Hmim) linkers in a sodalite-type topology, with the peculiarity of bridging zeolitic topologies with MOF-like tunability [8, 9]. Its remarkable thermal and chemical stability, combined with high specific surface area

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(SSA) and tunable porosity, have made it a key candidate for next-generation applications in gas capture, catalysis, sensing, and drug delivery [10–13]. ZIF-8 industrial relevance is confirmed by its commercial availability, marketed as Basolite Z1200 (BASF), priced at around 10 EUR/g [14]. However, its widespread growth remains hindered by the lack of sustainable and scalable synthetic routes. In the context of global transition towards green chemistry [15], ZIF-8 might be a valuable model system to explore how MOF synthesis can evolve from solvent-intensive lab-scale routes to truly sustainable and industrially viable processes [16].

ZIF-8 synthesis can be achieved using various techniques, ranging from traditional solvothermal and hydrothermal routes to advanced microwave, ultrasound, mechanochemical, and high-pressure methods. Nevertheless, among these approaches, the aqueous-based method stands out for its convenience, safety, and lower electricity costs [17]. Conventional ZIF-8 solvothermal synthesis, using zinc salts and Hmim as precursors, typically relies on organic solvents such as dimethylformamide (DMF) or methanol (MeOH). These enable high crystallinity and microporosity but raise serious concerns related to toxicity, economic, and environmental issues, including low reaction yields (20–30%), and the need for intensive solvent recovery [18–22].

A recent study reported the synthesis of ZIF-8 in an alternative solvent, glycerol carbonate, which proved highly effective, enabling the synthesis of mesoporous, highly crystalline materials [23]. A comparative life cycle assessment (LCA) [24, 25] study highlighted critical aspects of using this solvent compared to DMF, demonstrating that defining one pathway as more sustainable than another without a proper environmental assessment can lead to erroneous and misleading conclusions. In detail, the glycerol carbonate-based route could be competitive with that of DMF if its preparation involves waste cooking oil as glycerol source and dimethyl carbonate and MeOH, obtained as side-products, are recycled [26].

1.2 | Water as an Election Solvent for ZIF-8: the Greenest Solvent Overall

This tradeoff between material quality and environmental sustainability has driven research toward water-based routes, a highly desirable approach for ZIF-8 synthesis.

The aqueous synthesis of ZIFs has historically been challenging, due to the competition between framework nucleation and the precipitation of metal hydroxides or other amorphous phases, often yielding 1D or non-porous materials. Consequently, for a long time, it was assumed that the ZIF-8 phase could not form in purely aqueous systems. Successful crystallization in water requires a large excess of Hmim and a base to promote its deprotonation [19, 27, 28].

The first breakthrough came in 2011, when Pan et al. demonstrated that ZIF-8 could crystallize directly in water within minutes at room temperature, resulting in highly stable nanocrystals. This pioneering work proved that water could, in principle, replace DMF or alcohols in MOF synthesis. However, the method required a large excess of the organic linker (Zn:Hmim ratio of 1:70), raising doubts about its feasibility [29].

Building on this advance, a year later, Gross et al. introduced triethylamine (TEA) as a cobase to facilitate deprotonation and promote nucleation. This innovation dramatically reduced the linker excess (Zn:Hmim ≈ 1:4-16), enabling a rapid ZIF-8 formation at milder conditions with controlled particle sizes (60 ± 22 nm in diameter) but lower porosity (0.21–0.32 cm^3/g) and SSA (528–811 m^2/g) [30].

The subsequent optimization performed by Kida et al. further clarified the delicate balance between ligand concentration and framework purity, showing that ratios above 40 were necessary to suppress unwanted by-products such as $Zn(OH)_2$ and to achieve phase-pure ZIF-8. Under these conditions, their samples reached excellent textural properties (S_{BET} = 1400–1600 m^2/g, V_{pore} ≥ 0.60 cm^3/g) [31].

More recently, efforts have shifted towards methods that employ stoichiometric amounts of the precursors. In this context, Molina et al. achieved remarkable results, obtaining ZIF-8 using Zn:Hmim = 1:2 and TEA as the sole deprotonation agent, yielding highly crystalline materials under mild conditions (120°C, 14 h) and excellent reproducibility [32]. In parallel, Kim et al. demonstrated the first additive-free aqueous synthesis, scalable to multi-liter batches, bridging laboratory research with industrial applicability. In this case, the best synthesis of ZIF-8 in terms of highest crystallinity and narrowest size distribution was performed in 25 mL of water, with 1:10:406 molar ratio of Zn:Hmim: H_2O, in 15 min at 25°C. The same reaction was scaled up to a 2 L batch, leading to high yield (92%, 55 g of ZIF-8) and good structural properties of the final product, namely the SSA of 1094 m^2/g and micropore volume of 0.54 cm^3/g. These results show the efficiency of this green reaction upon scale-up, proving its significant potential in the field of ZIF-8 synthesis development [33].

Furthermore, ZIF-8 was generated at a pilot scale using a continuous hydrothermal synthesis approach in a flow reactor, employing water as the sole solvent to achieve a rapid, environmentally benign process and enable ZIF-8 synthesis at a production rate of 810 g/h [34]. ZIF-8 was also synthesized via a sonochemical approach under controlled pH conditions, employing aqueous NaOH together with a small quantity of TEA. Following optimization of the reaction parameters, the procedure was effectively scaled up to a 1 L synthesis, achieving an 85% yield at high substrate concentration (Zn^{2+}:DMF = 1:9.3) within 2 h while preserving the material's textural characteristics [35]. Another relevant work in this context was reported by Deacon et al. in 2022. Herein, nano-ZIF-8 was obtained through the ZIF-L synthetic pathway at a 10 L scale, resulting in the production of approximately 1 kg of nano-MOF with an 81% yield calculated relative to the zinc precursor [36].

In this context, Table 1 summarizes the main reaction conditions, yields, and textural properties reported for ZIF-8 syntheses in water solutions and DMF as bechmark.

From a climate change perspective, as adopted in a previous study, the water-based method—incorporating water at both the synthesis and washing stages—emerges as the most sustainable choice due to its lower global warming potential than organic alternatives [37].

In summary, these milestones show a remarkable evolution: from organic solvent-based syntheses requiring large chemical excesses of reagents to stoichiometric ratios, water-based, and scalable processes. Yet, despite these advances, the

TABLE 1 | Solvothermal synthesis of ZIF-8: main results.

Reference	Year	Zn:Hmim:H_2O molar ratio	Base	T, °C	t	Yield, %	SSA, m^2/g	V_{micro}, cm^3/g
Pan et al. [29]	2011	1:70:1238	—	25	5 min	80	1079	0.31
Gross et al. [30]	2012	1:16:2255	TEA	25	10 min	>95	811	0.32
Kida et al. [31]	2013	1:60:2228	—	25	1 h	94	1550	0.65
Molina et al. [32]	2024	1:2:450	TEA	25	20 h	97	1380	—
Kim et al. [33]	2024	1:10:406	—	25	15 min	92	1094	0.54
Tezerjani et al. [19]	2021	1:8:69 (DMF)	—	140	24 h	30	1370	0.51

environmental performance of all these routes, in terms of energy input, solvent management, and waste generation, remains largely unquantified.

Thus, understanding how synthesis parameters, solvent selection, and energy efficiency translate into environmental impact is crucial not only for ZIF-8 but also for the broader design of sustainable MOF manufacturing.

In this regard, the LCA methodology emerges as a powerful tool for quantifying the environmental performance of this promising synthetic route for ZIF-8.

2 | Materials and Methods

2.1 | Database and Software

The analysis utilized the *ecoinvent* database [38] (v.3.7.1) for all the background data. To account for the impacts related to average transportation distances, "market for" scenarios were taken into account, as these datasets represent all activities associated with a product within a specified region, including average transport and compensatory inputs for trade and transport losses.

The following geographical criteria guided the selection, given the international scope of the study, the global {GLO} provider was prioritized, choosing the European {RER} provider only when the {GLO} option was unavailable. The Allocation at Point of Substitution (APOS, U) model was selected as the allocation principle. This model is generally viewed as the most conservative approach, as it determines direct impacts based on physical flows, in contrast to methods such as consequential or cut-off procedures. The *SimaPro* software [39] (v. 9.2.0.2) served as the principal computational tool for executing the assessment. The harmonized life cycle impact assessment method *ReCiPe 2016* [40] was selected to quantify potential environmental effects. This methodology assesses impacts across 18 categories at the *midpoint* level, also known as the "problem-oriented" level.

The categories include global warming (GWP), stratospheric ozone depletion (SOD), ionizing radiation (IR), ozone formation human health (OF_HH), fine particulate matter formation (FPMF), ozone formation, terrestrial ecosystems (OF_TE), terrestrial acidification (TA), freshwater eutrophication (FE), marine eutrophication (ME), terrestrial ecotoxicity (TET), freshwater ecotoxicity (FET), marine ecotoxicity (MET), human carcinogenic toxicity (HCT), human noncarcinogenic toxicity (HNCT),

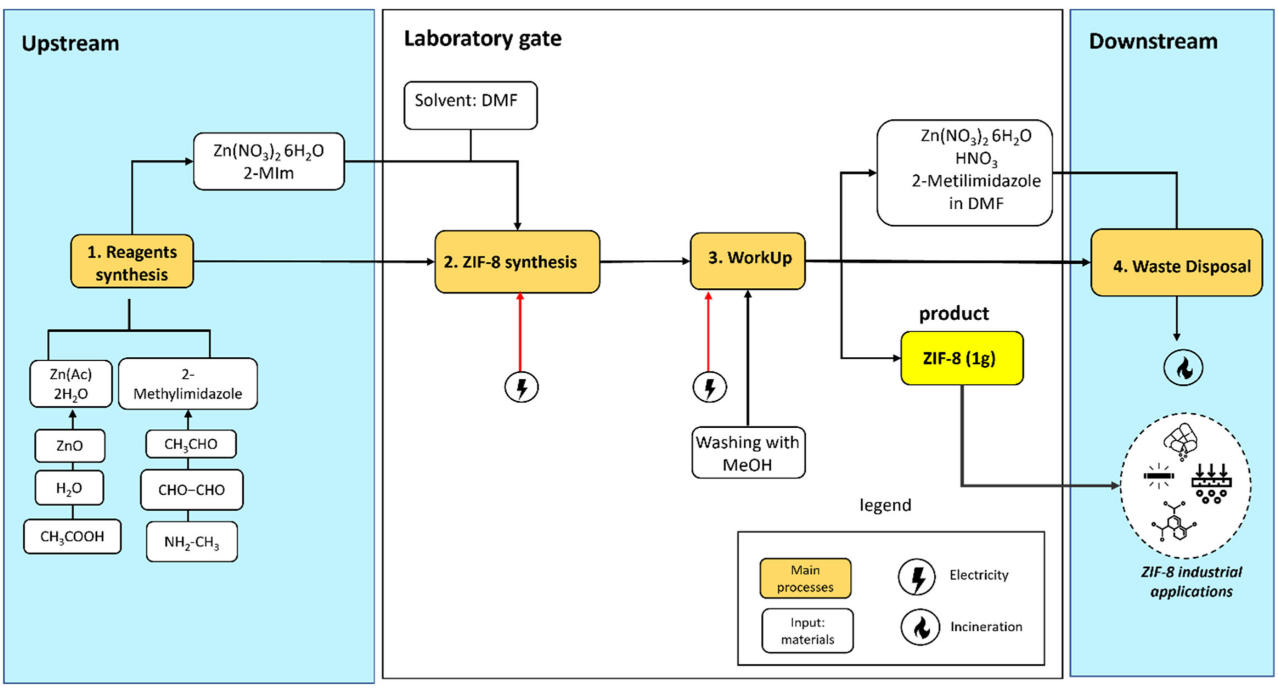

FIGURE 1 | DMF-based Scenario.

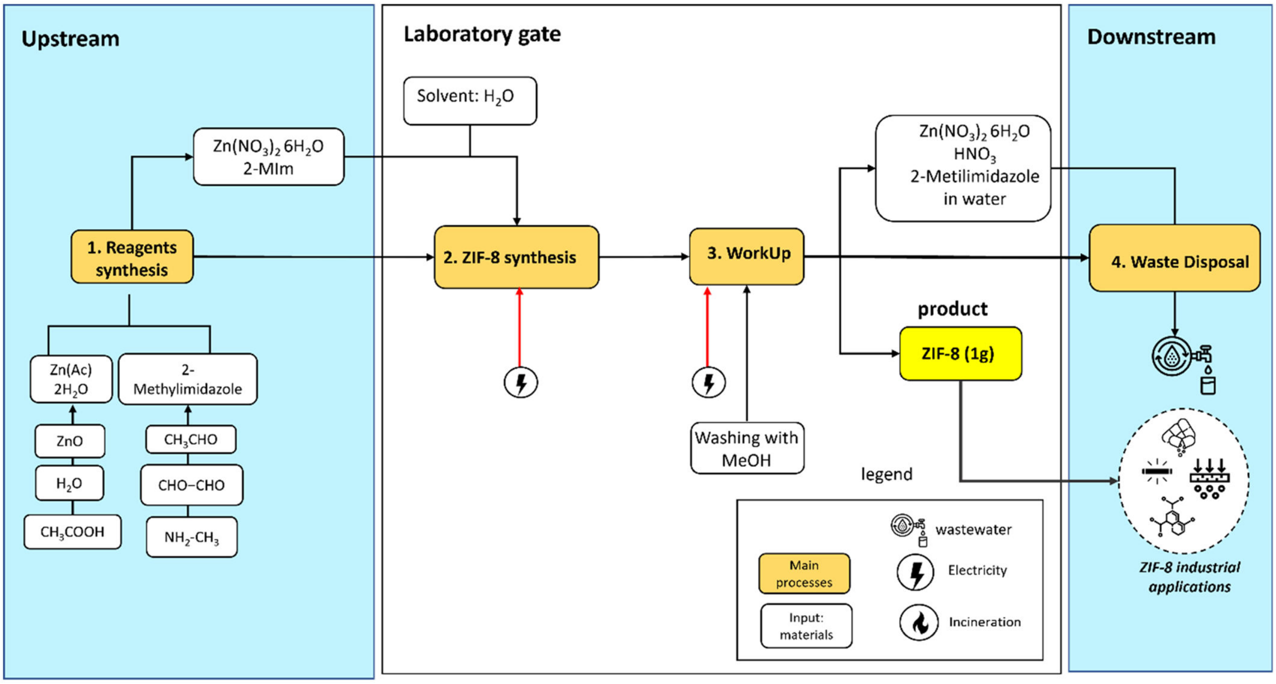

FIGURE 2 | Water-based Scenario.

land use (LU), mineral resource scarcity (MRS), fossil resource scarcity (FRS), and water consumption (WC). These categories can be further appropriately normalized and grouped into three *endpoint-damage* receptors: human health, ecosystem, and resource depletion. The endpoint method enables comparison of different processes based on a cumulative single score, here expressed in millipoint (*mPt*). Another useful tool used to assess environmental impacts was the *Cumulative Energy Demand* [41] (CED V1.11), which allows for the quantification of resource consumption (energy and raw material), by defining the renewable and non-renewable ones.

2.2 | Scenarios Description and Functional Unit

The water-based scenario (ZW) and DMF-based one (ZD) scenarios were thoroughly investigated along the whole processes from cradle to gate, consisting both of three main sections, as it is displayed in Figures 1 and 2: upstream (precursor's preparation), the set of operations within the laboratory gate (ZIF-8 synthesis, work-up) and waste disposal (wastewater for ZW, incineration for ZD).

Quantities were scaled to produce 1g of ZIF-8 (*functional unit*). All reactions were carried out using standard laboratory equipment. Since all the chemical processes discussed are performed using conventional laboratory apparatus, the entire energy requirement is assumed to be the only consumption of electrical power, excluding industrial-scale methods like recapturing waste heat or the direct utilization of factory steam. For quantifying energy usage, the standard power specification known as *Electricity*, *low voltage {GLO}, market group for, APOS*, *U* typical for laboratory equipment. Within this framework, the total electrical energy utilized (*kWh*) was derived by multiplying the device's power draw (*kW*) by its operational duration (*h*) [42]. A crucial step involved determining the instrument's power by accounting for its true functional temperature. Consequently, if a device was operated at a setting below its peak temperature, a compensatory multiplier, expressed as the ratio ΔTworking/ΔTmax was introduced [43].

3 | Results and Discussion

3.1 | LCA as a Robust Methodology to Indicate a More Sustainable Synthetic Route

In this work, we offer a critical discussion of the efficacy and sustainability of the laboratory-scale aqueous synthesis route for ZIF-8.

The current analysis is quantitatively grounded in a comparative LCA, which serves to rigorously delineate the environmental advantages and tradeoffs of the water-based methodology when it is compared to the conventional DMF-based method within their whole production framework (from cradle to gate). The importance of using a benchmark to compare results within the green chemistry sector has also been highlighted recently as one of the 12 fundamental principles for the LCA of chemicals [44]. Building on the empirical findings of this work and extant literature, we further present critical perspectives and projections concerning the expected environmental implications inherent in transitioning this synthetic methodology to industrial-scale production.

The scenario employing water as a solvent was built using foreground data from Kida's work [31], while the DMF-based scenario was designed by importing data from Tezerjani's insights [19]. Materials and energy flows of the two processes are depicted in Figures 1 and 2, while the full inventories are reported in the S2 paragraph. Additionally, energy consumption details are listed in section S3.

TABLE 2 | Results per impact category for the two investigated scenarios ZD and ZW at midpoint level (ReCiPe 2016 Midpoint H).

Impact category	Unit	ZD	ZW
GWP	*kg CO_2 eq*	7.96	1.11
SOD	*mg CFC11 eq*	0.00330	0.000475
IR	*kBq Co-60eq*	0.945	0.132
OF HH	*mg NO_x eq*	16.8	2.34
FPMF	*mg PM2.5 eq*	16.9	2.31
OF TE	*mg NO_x eq*	16.8	2.34
TA	*mg SO2 eq*	26.0	3.66
FE	*mg P eq*	3.88	0.534
ME	*mg N eq*	0.455	0.0780
TET	*kg 1,4-DCB*	1.24	0.178
FE	*g 1,4-DCB*	13.3	1.88
ME	*g 1,4-DCB*	19.2	2.70
HCT	*g 1,4-DCB*	1.45	0.949
HNCT	*g 1,4-DCB*	60.6	10.1
LU	*m^2 crop eq*	0.340	0.0493
MRS	*mg Cu eq*	5.10	0.816
FRS	*kg oil eq*	2.04	0.312
WC	*dm^3*	60.5	9.30

Abbreviations: FE, freshwater eutrophication; FET, freshwater ecotoxicity; FPMF, fine particulate matter formation; FRS, fossil resource scarcity; GWP, global warming potential; HCT, human carcinogenic toxicity; HNCT, human noncarcinogenic toxicity; IR, ionizing radiation; LU, land use; ME, marine eutrophication; MET, marine ecotoxicity; MRS, mineral resource scarcity; OF_TE, ozone formation terrestrial ecosystems; OF_HH, ozone formation, human health; SOD, stratospheric ozone depletion; TA, terrestrial acidification; TET, terrestrial ecotoxicity; WC, water consumption.

As a first evaluation, the water-based scenario (ZW) was compared with the DMF-based one (ZD) in terms of their environmental performances across all the 18 problem-oriented impact categories provided by ReCiPe 2016 [40], giving an immediate and comprehensive assessment of each scenario. The results are presented in Table 2.

A quick glance at the table reveals the following trend: across all categories, the ZW scenario has the lowest impact relative to ZD, generally ranging from 83.2% to 86.3%, except for the HCT category, where the percentage reduction is 34.5%. A contribution analysis for all the investigated impact categories is reported in Figure 3, highlighting the prominent contribution of energy consumption in both investigated scenarios (with the exception of ME and HCT for ZW where 2-methylimidazole is the predominant contributor).

Within this context, as also outlined in literature [45], LCA applied to lab-scale data inherently presents significant opportunities for optimization. Specific environmental impacts, most notably those associated with electricity consumption, are expected to undergo a reduction at larger scales due to the realization of improved process efficiencies and inherent economies of scale.

At larger scales, technological shifts, fluctuating pricing dynamics, and evolving regulatory frameworks may concurrently lead to variations in both the environmental and economic outcomes. These inherent uncertainties collectively make it challenging to produce entirely realistic industrial-scale simulations. Nevertheless, the systematic consideration of these factors remains crucial, as it substantially enhances the prospective accuracy of the modeled scenarios [46].

Since what was just discussed, an additional contribution analysis was proposed, but this time excluding the overall energy consumption (Figure 4). This also allows the punctual identification of the other contributors, expecting a distribution of impacts more like the actual one observed on a larger scale, as reported in the reference work [47].

Once the high-energy consumption effects are excluded, it is possible to estimate the distribution of the impacts through only the involved materials for each process stage (in terms of their required mass). For the ZW scenario, a relevant contribution comes from the use of 7Hmim, which is classified as toxic due to its potential risks to human health, and this finding is also consistent with a previous study [47].

Otherwise, regarding ZD, the overall distribution of the impacts appears to differ slightly from that obtained and reported in a

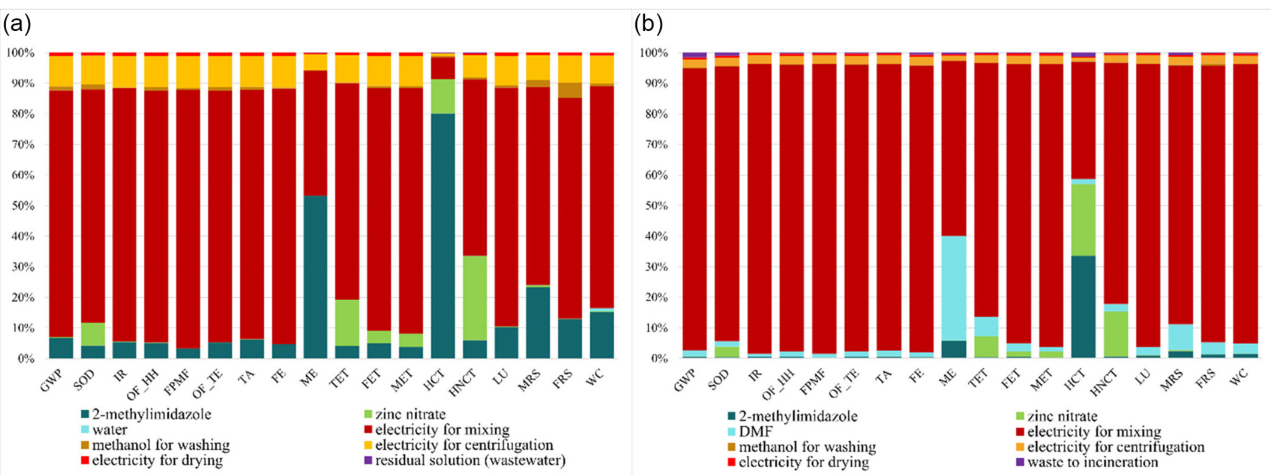

FIGURE 3 | Contribution analysis for (a) ZW and (b) ZD scenarios (%) obtained through the ReCiPe 2016 Midpoint (H) method.

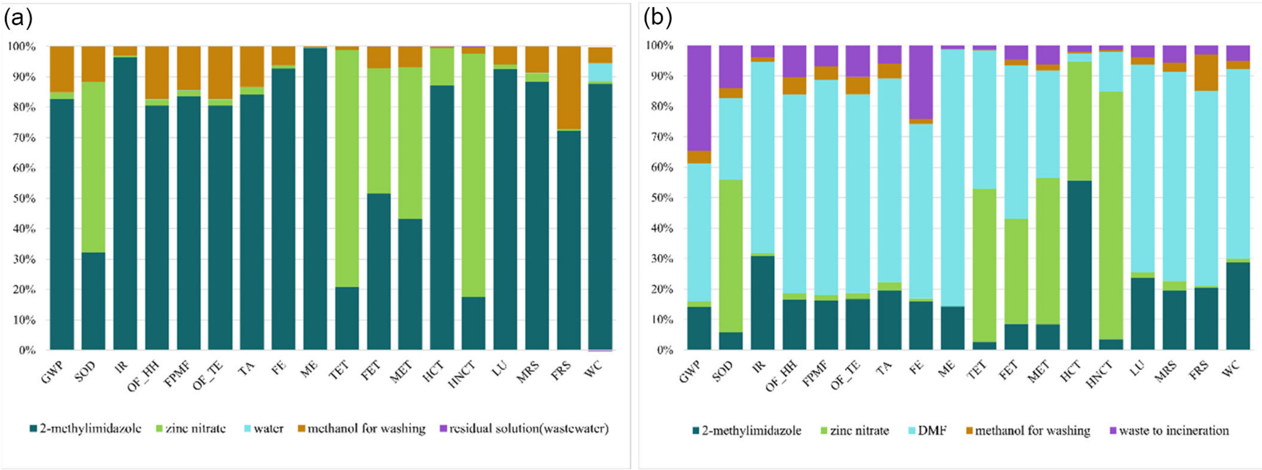

FIGURE 4 | Contribution analysis for (a) ZW and (b) ZD scenarios, excluding the overall energy consumption, (%) obtained through the ReCiPe 2016 Midpoint (H) method.

previous work [471]. In both cases, the solvent employment itself brings relevant impacts, but in literature also a major effect is given by the washing step, carried out in DMF instead of MeOH (as carried out in this work), since two different works are taken in account (literature analysis is based on data imported from Park et al. study [18], while our work refers to Tezerjani et al. findings [19]).

Furthermore, there are several key differences compared to the benchmark literature work [47]. The functional unit is 1 kg of ZIF-8, whereas in our case, it is 1 g, closer to the actual laboratory-scale scenario. This disparity has several implications, including a different profile of energy consumption due to the scale difference. Additionally, WC is consistently ignored in the aforementioned study. The power consumption for the vacuum oven (operated at room temperature) and the centrifuge is also disregarded, and the literature article does not consider the waste generated during the ZIF-8 production process. Finally, the electricity provider in the literature study was set to that of Malaysia [47].

When shifting towards the endpoint approach, the same general trend is observed: a reduction is noted when transitioning from the ZD scenario (486 mPt) to the ZW scenario (52 mPt), as displayed in Figure 5. In both cases, the human health receptor category is the most significantly affected [47], primarily dependent on energy consumption (electricity), accounting for 73 % and 83 of the impact (referring to human health damage) in the ZD and ZW scenarios, respectively. If we exclude the impact of electricity consumption (Figure 5b), a reduction of 98% and 93% on the total impacts is observed. The ZD scenario remains dominated by human health impacts, while ZW also shows a notable impact on ecosystems, due to both Hmim and employment of MeOH during the washing step.

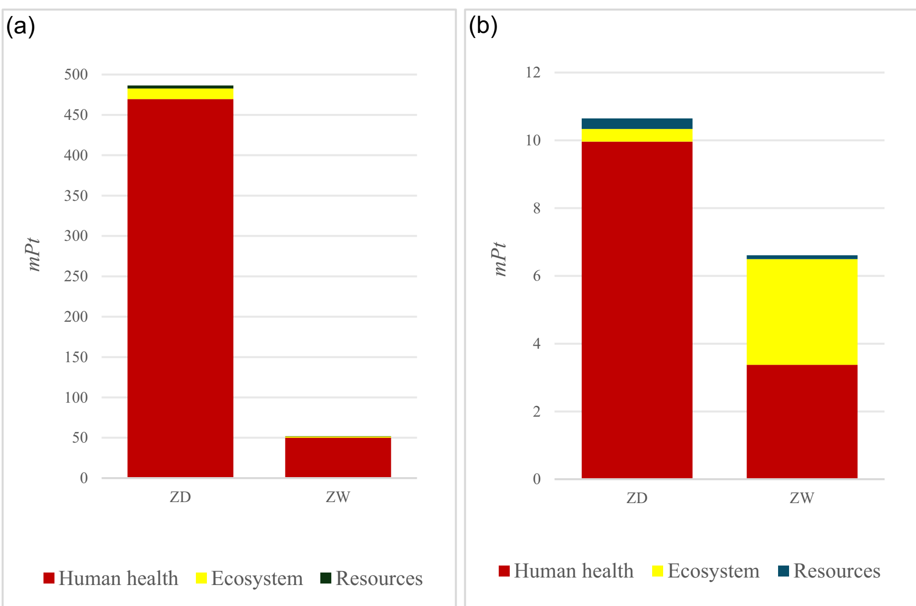

FIGURE 5 | Life cycle impact assessment (LCIA) of ZD and ZW (a) including total energy consumption and (b) excluding total energy consumption, obtained through the ReCiPe 2016 EndPoint (H) method.

Once the energetic contributions are excluded, the impact of the remaining elements and reactants can be evaluated in terms of mass (Figure 6). In fact, in the case of ZD, a large contribution came from the solvent itself (57% on total), while for ZW the Hmim has a noticeable impact (79%), given the large excess with which it is used, while water contribution is negligible.

Another key indicator is the CED [4], it enables precise resource identification and distinguishes between the two main categories based on origin: renewable and nonrenewable resources expressed then in the form of energy equivalent values. The analysis (Figure 7a) shows that the total CED is 128 MJ for ZD, while it is 44 MJ for ZW, suggesting a still high reliance on fossil resources for both cases.

If electricity is excluded, the trend would be *reversed*, resulting in a higher CED value for the water scenario (Figure 7b), as water-related impacts would be higher due to wastewater generation resulting from the significant excess of water used to carry out the reaction (Detailed LCIA results are provided in Section S4 of the Supplementary Information).

A data "Pedigree matrix" [48] was used to determine the uncertainty ranges for the inventory data related to reagents, energy input, and waste streams. This matrix attributes data quality scores on a scale ranging from 1 (best) to 5 (worst), based on several parameters that may influence a method's reproducibility and robustness. These parameters are data representativeness, acquisition methods, and correlations across time, technology, and geography. Furthermore, the standard deviation (SD) of input and output data for each process was determined using the data quality pedigree matrix, and values are reported in Table S12. The lognormal statistical distribution was selected for the calculation, with a 95% confidence interval.

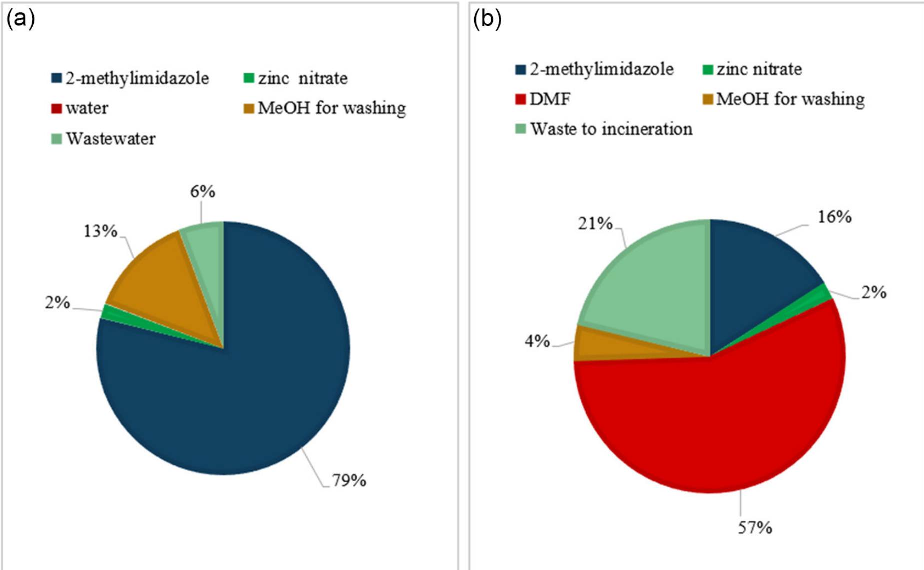

FIGURE 6 | Contribution analysis for water-based (a) and DMF-based (b) scenarios excluding the overall energy consumption, (%) obtained through the ReCiPe 2016 EndPoint (H) method.

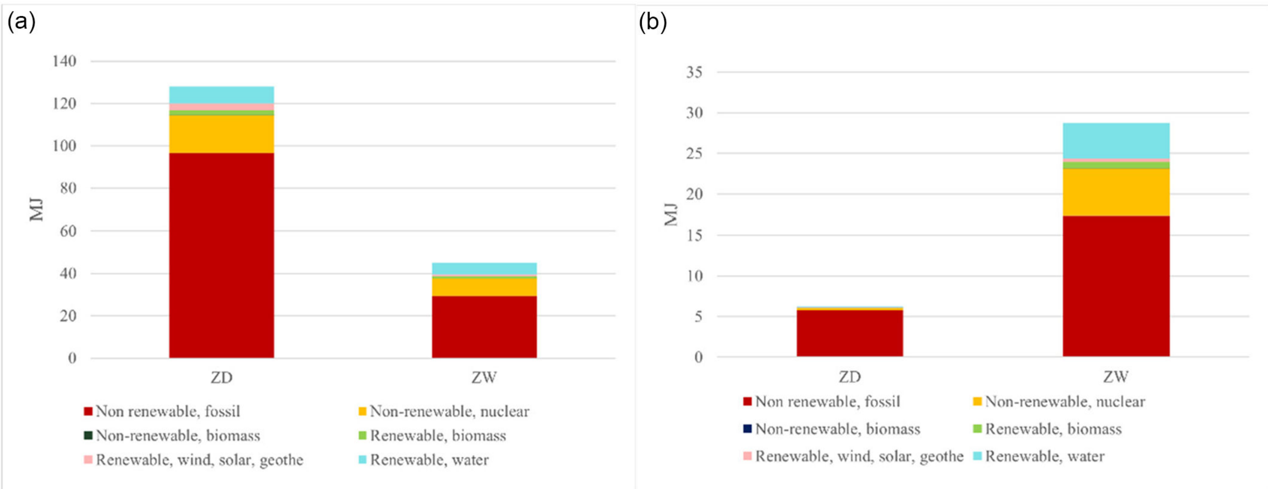

FIGURE 7 | Total primary energy distribution expressed in MJ for DMF-based and water-based scenarios (ZD, ZW) (a) including the overall energy consumption and (b) excluding the overall energy consumption, obtained through the Cumulative Energy Demand v.1.11 method.

The Monte Carlo simulation was applied to the scenarios to provide a proper uncertainty analysis, by reiterating the comparison for 1.000 runs. Results expressed through the cumulative single score (endpoint) showed that for more than the 99% of cases (Figure S1 of the SI), the ZW scenario appears to be the most advantageous one in terms of environmental impacts when compared to ZD. In fact, green bars represent the simulations resulting in ZD > ZW, indicating the scenarios where ZD carries a greater environmental burden than ZW.

4 | Conclusions and Future Perspectives

The LCA study clearly highlights that the water-based synthesis of ZIF-8 is more sustainable when compared with other solvothermal preparation routes. In fact, the LCIA shows a lower environmental impact, with a reduction of at least 83% across all impact categories except one, when compared to synthesis in DMF. Consistent with previous LCA-based investigations, water emerges as the solvent of choice also when compared with alcohols such as MeOH [49]. Aqueous conditions favor the preparation of microporous ZIF-8, similarly to what is observed for DMF- and alcohol-based syntheses. Based on the results, future studies on the solvothermal preparation of ZIF-8 should prioritize water as the solvent. Indeed, mild reaction conditions, high yields, and excellent textural properties make water the most sustainable option. Temperature, reagent concentration, pouring time, reactant ratio, stirring rate, and preparation method are crucial parameters that must be tuned to obtain ZIF-8 with the desired particle size and size distribution. These parameters directly affect nucleation and crystal growth processes. In this context, a recent study reports a large-scale synthesis of 2 L of ZIF-8 with a narrow particle size distribution, resulting in enhanced adsorption performance for methylene blue removal from aqueous solutions [33]. Further studies are therefore required to extend the scalability of ZIF-8 synthesis in water. From an LCA perspective, there is ample scope to expand the application of this methodology to compare ZIF-8 use in specific applications (e.g., CO_2/CH_4 separation) or to benchmark ZIF-8 against alternative materials, such as other MOFs or zeolites. Additionally, ZIF-8 materials with different porosities and particle size distributions synthesized in water are of interest to broaden their application fields and better identify the most suitable material characteristics for specific purposes [50]. The ZIF market is projected to reach USD 3.5 billion by 2033, growing at a compound annual growth rate of 15.5% from 2026 to 2033 (ZIF-8 accounting for over 35% of the total market) [51]. A techno-economic analysis would be useful to obtain quantitative insights into production costs, scalability, energy and solvent demands, and supply-chain constraints, thereby guiding material selection, process optimization, and the transition of ZIF-based technologies from laboratory scale to industrial implementation.

Acknowledgments

R.C. is grateful to University of Salerno for research fund “FARB” (ORSA252349) and to Italian Ministry of University and research (MUR) for FISA-2023- 00132 project “ALTEREGO - ALuminum wasTEs recYcling and valoRisation for Environmentally friendly GOals” - Area “Advanced Materials” (CUP D43C23004630001).

Open access publishing facilitated by Universita degli Studi di Salerno, as part of the Wiley - CRUI-CARE agreement.

Funding

This study was supported by Università degli Studi di Salerno (ORSA252349), Ministero dell'Università e della Ricerca (CUP D43C23004630001).

Conflicts of Interest

The authors declare no conflicts of interest.

Data Availability Statement

The data that supports the findings of this study are available in the supplementary material of this article.

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Supporting Information

Additional supporting information can be found online in the Supporting Information section.