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Mapping the Research Landscape of Zeolitic Imidazolate Frameworks (ZIFs) for Hydrogen Production: Structural Modelling and Bibliometric Analysis

Juan Matmin[a,b,e*], Siti Nur Umairah Shikh Mohd Fauzi[a], Khairul Rijal Razali[a], Nur Hikamah Seth[a], Mohamad Hamdi Zainal-Abidin[a], Nik Ahmad Nizam Nik Malek[b,c], Aishah Abdul Jalil[d], Susilawati Toemen[a], Mohd Izzam Idrus[e]

[a] Department of Chemistry, Faculty of Science, Universiti Teknologi Malaysia, 81310 UTM Johor Bahru, Johor, Malaysia.
[b] Centre for Sustainable Nanomaterials, Universiti Teknologi Malaysia, 81310 UTM Johor Bahru, Johor, Malaysia.
[c] Department of Biosciences, Faculty of Science, Universiti Teknologi Malaysia, 81310 UTM Johor Bahru, Johor, Malaysia.
[d] Centre of Hydrogen Energy, Institute of Future Energy, Department of Chemical Engineering, Faculty of Chemical and Energy Engineering, Universiti Teknologi Malaysia, 81310 UTM Johor Bahru, Johor, Malaysia.
[e] Bangunan T03, Universiti Industry Research Laboratory (UIRL), Pusat Pengurusan Makmal Universiti (PPMU), Universiti Teknologi Malaysia, 81310 UTM Johor Bahru, Johor, Malaysia.

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*Corresponding author
juanmatmin@utm.my

Abstract

Zeolitic Imidazolate Frameworks (ZIFs) have gained significant attention as potential catalysts for the Hydrogen Evolution Reaction (HER), a critical process in sustainable hydrogen production. This review offers an in-depth examination of ZIFs, emphasizing how their structural versatility—through the selection of metal centers and organic linkers—directly impacts HER efficiency. We analyze key ZIF-based catalysts, highlighting their performance in terms of electron transfer, active site exposure, and stability under reaction conditions. A bibliometric analysis tracks the growth of research in this domain, revealing collaboration networks and identifying the most influential studies driving innovation. By mapping the research landscape, we uncover trends, challenges, and emerging areas that are shaping the future of ZIFs in HER. The integration of structural modelling and bibliometric analysis provides a holistic understanding of the progress made in this field and serves as a guide for future research efforts aimed at optimizing ZIFs for hydrogen generation. This review underscores ZIFs' pivotal role in advancing the hydrogen economy through efficient HER processes.

Keywords Zeolitic imidazolate frameworks, molecular modelling, bibliometric analysis, hydrogen production, water splitting

1.0 INTRODUCTION

The global energy landscape is rapidly evolving, with hydrogen emerging as a critical component in sustainable energy systems. Often referred to as the “fuel of the future,” hydrogen is at the forefront of the transition to clean energy. Its versatility

as an energy carrier, with applications in fuel cells, energy storage, and green chemical production, has fuelled extensive research and innovation. As the world aims to reduce carbon emissions and increase energy efficiency, sustainable hydrogen production has become an urgent priority. This challenge has led to the development of advanced materials, with zeolitic imidazolate frameworks (ZIFs) standing out as particularly promising for enhancing hydrogen production processes.

ZIFs, a specialized subclass of metal-organic frameworks (MOFs), are known for their high surface area, tunable pore structures, and remarkable chemical stability. These properties make them ideal candidates for catalytic applications, especially in the hydrogen evolution reaction (HER) and water splitting, two essential processes for clean hydrogen production. By customizing their structures, researchers can optimize ZIFs to boost hydrogen production efficiency, paving the way for scalable, sustainable energy solutions. Recent studies demonstrate that ZIFs' ability to catalyze reactions under challenging conditions offers significant potential to overcome the limitations of existing hydrogen production technologies (Pan et al., 2012; Zafari et al., 2023).

Water splitting, which consists of the HER and the oxygen evolution reaction (OER), requires effective catalysts to reduce the energy barriers of these processes. While noble-metal catalysts like platinum (for HER) and iridium oxide (for OER) are highly efficient, their cost and scarcity have spurred research into alternative materials. ZIFs, constructed from transition metals like zinc or cobalt linked by imidazolate ligands, have attracted significant attention due to their high chemical stability, large surface area, and adjustable porosity. While ZIFs share structural similarities with zeolites, their greater flexibility in functionality and modification makes them promising candidates for catalytic applications. To fully harness their potential for hydrogen production, however, we need to delve deeper into how structural factors influence their catalytic performance. Additionally, a comprehensive understanding of the broader research landscape, including publication trends, collaborations, and emerging themes, is essential. This review aims to comprehensively examine ZIFs for hydrogen production through both structural modelling and bibliometric analysis, identifying key trends, challenges, and future directions.

The first section of the review focuses on structural modelling. Using computational and theoretical methods, we can predict and enhance ZIFs' performance in hydrogen production. Likewise, ZIFs are composed of transition metal ions (such as Zn, Co, and Fe) coordinated by imidazolate linkers, forming zeolite-like structures. Fine-tuning these frameworks can improve their catalytic properties, increasing the efficiency of hydrogen production. ZIF-8, for example, with its sodalite topology, is notable for its high thermal stability and large internal cavities, which enhance hydrogen adsorption and reactivity (Huang et al., 2023). Understanding these structural features is key to advancing ZIFs' role in sustainable hydrogen production. The second section of the review presents a bibliometric analysis to track major trends and patterns in ZIF-hydrogen research. By analyzing publications, citation networks, and global collaborations, this section highlights influential studies and leading research hubs. It offers insight into the evolution of the field, identifies knowledge gaps, and reveals opportunities for future research. The analysis also sheds light on the collaborative networks driving advancements in ZIF-based hydrogen production technologies (Fernández-Castro et al., 2021).

In conclusion, this review provides a comprehensive overview of ZIFs' role in hydrogen production, combining structural insights with a bibliometric analysis. By identifying key trends and challenges, it charts a path for future research, advancing both the science and application of ZIFs in clean energy technologies. The insights gained from this review will help fuel innovation and meet the growing global demand for sustainable hydrogen solutions.

2.0 STRUCTURAL MODELLING OF ZEOLITIC IMIDAZOLATE FRAMEWORKS (ZIFs)

In this study, HyperChem 8.0 was used to determine the properties of the molecules by analyzing the energy parameters such as bond length and bond angle of crystalline structure zeolites framework. For the ease of representation on ZIFs structures, ZIF-8 compounds containing 100 atoms were analyzed using density functional theory (DFT) and 6-31G as the minimum basis set. Initially, before adding Zn into nitrogen at the 2-MeIM compound, the bond angle for the sp^2 hybrid of N1-C2-N3 was 111.46° (Hachula et al., 2010) as shown in Figure 1 (a). The value of the bond angle stated was slightly smaller than the predicted value of sp^2 hybridization, which is 120°. This difference is caused by the presence of lone pairs of electrons on the N3 atom. The orbitals occupied by lone pairs are shorter and rounder than those occupied by bonding pairs. As a result, a lone pair and a bonding pair repel each other more than two bonding pairs repel each other, significantly compressing the bonding pairs and lowering the bond angle from 120° to 111.46°. However, the addition of zinc forms a metal-imidazolate-metal connection with a bond angle of 145° (Pan et al., 2018), as shown in Figure 1 (b). This change in bond angle may be due to the loss of lone pairs on the N3 atom, which eliminates the repulsion between N1-C2-N3 molecules.

The length parameters were based on CH_4 molecules being positioned about 3.4 Å away from each imidazole ring due to van der Waals repulsion from hydrogen atoms (Yu et al., 2021). The CH_4 molecules shift in position based on DFT calculations, forming either a vertex or triangle shape at the aperture. As seen in Figure 1 (c), the CH_4 molecules alternate between these two shapes, creating the pristine ZIF-8 structure. The C2–C21 long bond represents the size of the 6-membered ring gate, which is approximately 3.4 Å in diameter. In ZIF-8, the most important structural features are the N–Zn

bond, the N–Zn–N angle, and the C2–C2 long bond. Based on the specified conditions, the structural arrangement of bonds existing in 2-MeIM and ZIF-8 is shown in Figure 1.

The tetrahedral compound and bridging oxygen atoms present in zeolites are based on divalent M–Im–M structures (M = Zn, Co, and Im = imidazole or methylimidazole (2-MeIM) linkers, as illustrated in Figure 1 (a)). On the other hand, one Zn atom and four imidazolate linkers with a tetrahedral structure form the basic structure of ZIF-8, as illustrated in Figure 1 (d). The compound formed using HyperChem had good agreement with the structure described by Zheng et al. (2016). This shape includes N–Zn bonds and N–Zn–N angles corresponding to a hybrid structure with both organic and inorganic components. However, in ZIF-8, these interactions are considered weak, preventing the addition of compounds into the crystal (Zheng et al., 2016). Hence, by using the same basic compound, we constructed a 6-membered ring (6MR) with more firm flexibility, showing a more crystalline structure of ZIF-8 (Benedetti et al., 2020). The existence of square and hexagonal windows surrounding the main pore characterizes the stable sodalite ZIF-8 crystal (Figure 1 (e)).

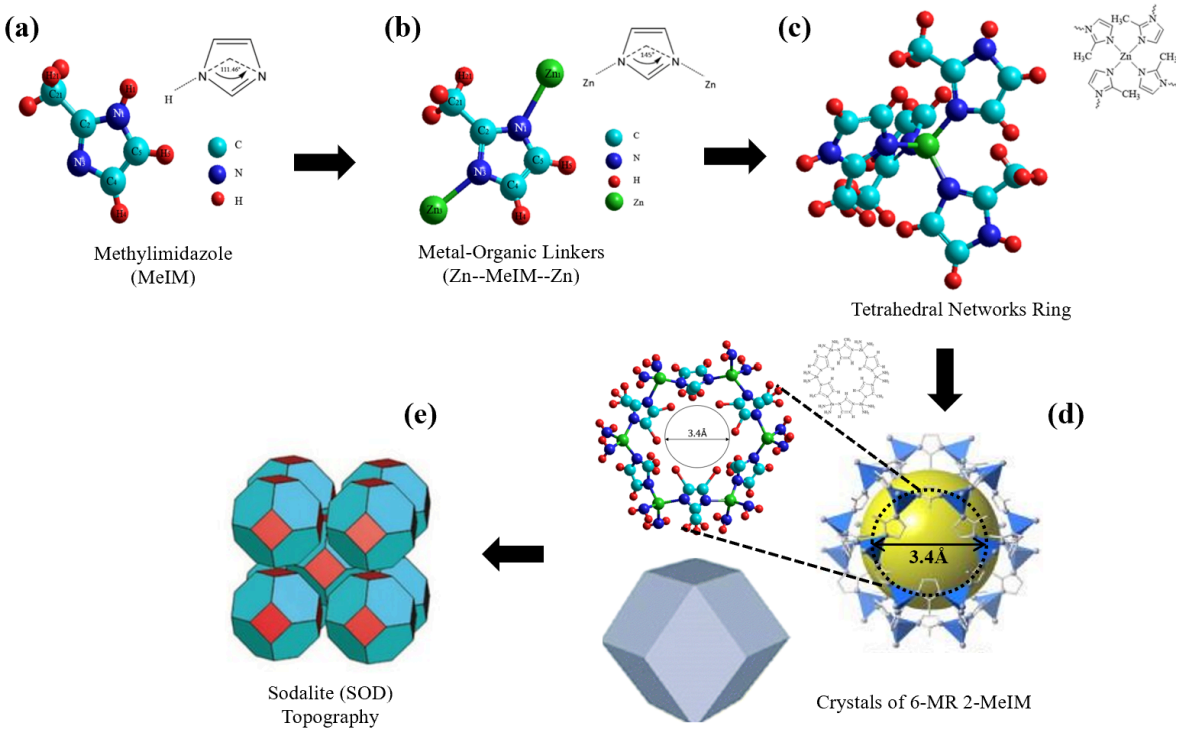

Figure 1 Molecular modelling based on HyperChem 8.0 for (a) 2-MeIM, (b) Metal-Organic Linkers (where M = Zn), (c) Tetrahedral networks ring, (d) Formation of ZIF-8 crystal by 6-MR, 2-MeIM, and (e) Sodalite topography structures.

Table 1 compares the bond length parameters of 2-methylimidazole (2-MeIM) and the ZIF-8 framework, showing that most bond lengths are identical between the two, including N1-C2 (1.3474 Å), N1-C5 (1.3700 Å), N3-C2 (1.3270 Å), N3-C4 (1.3840 Å), C4-C5 (1.3560 Å), C2-C21 (1.5009 Å), C4-H4 (1.1021 Å), C5-H5 (1.1021 Å), and C21-H21 (1.1127 Å). However, the N1-Zn1 bond in ZIF-8 is longer (0.9900 Å) than in 2-MeIM (0.8700 Å), likely due to zinc coordination. Bond lengths depend on bond order—higher bond order results in shorter bonds. In 2-MeIM, the shortest bond is N1-H1, while the longest is C2-C21. The asymmetry between N3-C2 and N1-C2 is typical in imidazole derivatives, with the N3-C2 double bond being shorter (1.327 Å) and stronger than the N1-C2 single bond (1.347 Å), as seen in Table 1. This is supported by previous research (Hachula et al., 2010). In ZIF-8, the N1-H1 bond is replaced by N1-Zn1, with little change in bond length due to similar bond order. The longest bond in both ZIF-8 and 2-MeIM is C2-C21 (1.5009 Å), consistent with its single bond nature, as shown by HyperChem 8.0 calculations. Additionally, the length parameters for ZIF-8 were influenced by CH_4 molecules positioned about 3.4 Å from each imidazole ring due to van der Waals repulsion (Yu et al., 2021). CH_4 molecules shift between vertex and triangle shapes at the aperture, as seen in Figure 1 (d), contributing to the formation of the ZIF-8 structure. Key structural features in ZIF-8 include the N–Zn bond, the N–Zn–N angle, and the C2–C21 bond, with the 6-membered ring gate measuring approximately 3.4 Å.

Table 1 Bond length parameters of 2-MeIM and ZIF-8 frameworks.

Bond Type	Bond Length Å (2-MeIM)	Bond Length Å (ZIF)
N_1-C_2	1.3474	1.3474
N_1-C_5	1.3700	1.3700
N_1-Zn_1	0.8700	0.9900
N_3-C_2	1.3270	1.3270
N_3-C_4	1.3840	1.3840
C_4-C_5	1.3560	1.3560
C_2-C_{21}	1.5009	1.5009
C_4-H_4	1.1021	1.1021
C_5-H_5	1.1021	1.1021
C_{21}-H_{21}	1.1127	1.1127

As proved by structural modelling analysis, ZIFs are constructed from tetrahedrally coordinated metal ions, like Zn or Co, linked by imidazolate groups, creating a highly porous structure. The flexibility in metal coordination and organic linkers enables precise control over ZIFs' structural and chemical properties. This adaptability, along with consistent bond lengths and stable frameworks, makes ZIFs particularly effective for catalytic applications, such as hydrogen evolution reactions (HER) and water splitting. Their tunable surface areas and bond configurations help lower the overpotential required for HER. Studies show that ZIFs, either on their own or combined with metals or other nanomaterials, enhance catalytic performance. Nowadays, metal-doped and hybrid ZIFs exhibit significant improvements in HER efficiency, demonstrating their potential in energy-related applications. The effectiveness of ZIFs materials greatly influences their performance in the HER. ZIFs compounds with structures such as ZIF-8 demonstrate chemical and heat resistance that is essential in challenging HER environments. The robust structure of ZIFs materials helps them withstand degradation over cycles while sustaining a level of catalytic performance. Metal ions, like zinc and cobalt are crucial in ZIFs frameworks as they facilitate electron transfer and expose sites effectively. The durability of these frameworks enables function by preventing degradation and preserving porosity. Additionally doping or combining ZIF with substances could strengthen their durability and conductivity resultantly enhancing the efficiency of the hydrogen evolution reaction. Today, researchers are investigating combining ZIFs with nitrogen doped carbons or graphene to enhance both stability and catalytic capability. The significance of crafting ZIFs structures, with customized durability is emphasized to enhance their efficiency, in hydrogen production methods.

3.0 BIBLIOMETRIC ANALYSIS OF ZEOLITIC IMIDAZOLATE FRAMEWORKS (ZIFs)

In this study, the bibliometric analysis was conducted using the Scopus database, with VOSviewer employed to create visual maps of the research landscape, highlighting key publications, authors, keywords, and citation networks. We explored the intersection MOFs and hydrogen production through water splitting by utilizing a structured query in Scopus. This query included titles, abstracts, and keywords related to “Metal Organic Frameworks,” “zeolitic imidazolate frameworks,” “hydrogen,” and “water splitting,” ensuring a comprehensive capture of relevant literature. Subject areas were refined to include Chemistry, Materials Science, Chemical Engineering, Energy, Biochemistry, Environmental Science, Engineering, Physics, and Multidisciplinary Studies, reflecting the interdisciplinary nature of the research. The analysis focused on articles and reviews to provide in-depth insights into current trends, while restricting results to English-language publications for broader accessibility. The initial search yielded 1,242 publication records, highlighting a substantial body of literature dedicated to exploring MOFs and their applications in sustainable hydrogen production. This substantial yield lays the groundwork for a detailed bibliometric analysis of trends and influential works in the field.

It is worth mentioning that Scopus was chosen as the database for bibliometric analysis due to its comprehensive coverage of high-impact journals across diverse fields, including Chemistry, Materials Science, and Energy. Its structured query features allow for refined searches using titles, abstracts, and keywords, ensuring a robust dataset for bibliometric studies. Additionally, its emphasis on peer-reviewed content provides a reliable foundation for analysis. VOSviewer was selected for its unique ability to visualize bibliometric data through co-authorship, keyword co-occurrence, and citation networks. Its strength lies in creating clear and interactive visual maps that highlight clusters of research focus, emerging trends, and influential contributors. The combination of these tools supports a thorough and visually interpretable analysis of the research landscape surrounding ZIFs and their applications in hydrogen production.

The bibliometric analysis depicted in Figure 2 provides an insightful overview of the research landscape for HER and MOFs. One of the most notable clusters is the central role of ZIFs in HER-related research. ZIFs hold a prominent and central position in the bibliometric network, underscoring their critical role in advancing HER technology, as shown in Figure 2(a). In

Figure 2(b), the keywords co-occurrence cluster associated with the ZIFs pattern is densely connected to other key concepts such as “metal-organic frameworks,” “hydrogen evolution reaction,” and “catalyst,” indicating their versatility and broad applicability (Li et al., 2021). This suggests that research in this area is converging on catalytic applications, particularly in hydrogen evolution.

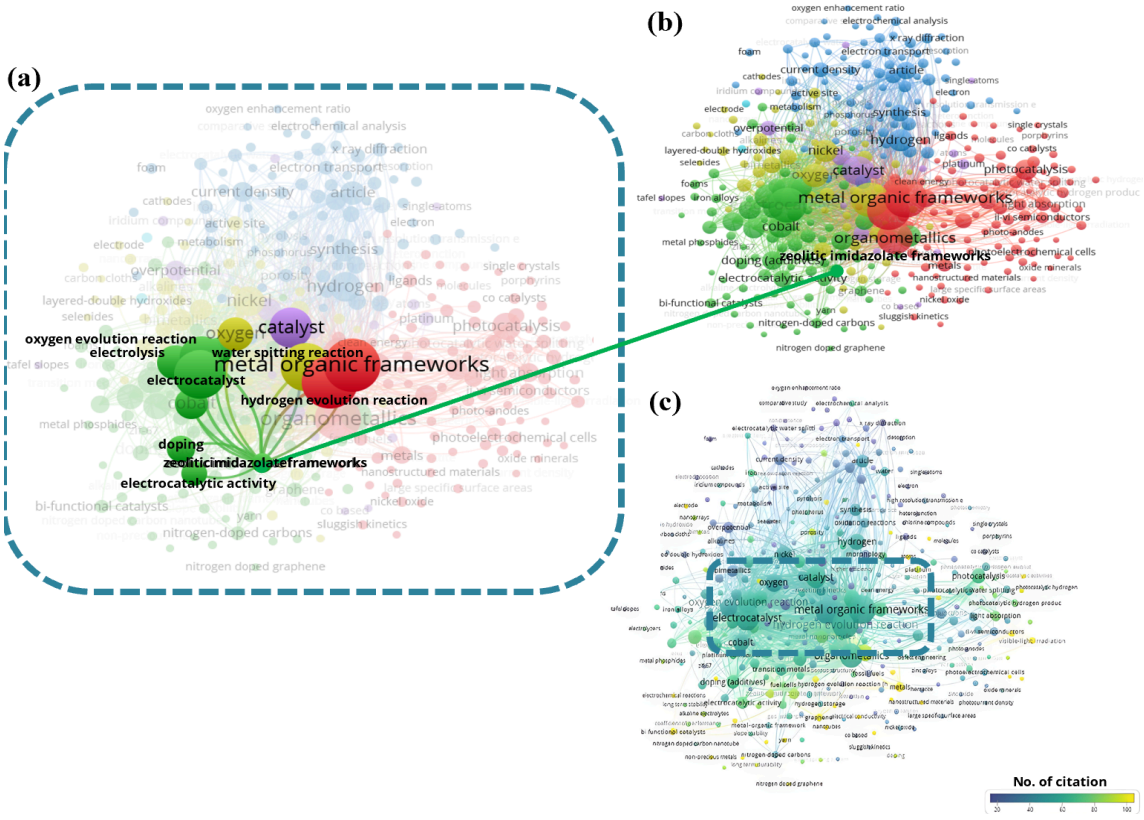

Figure 2 Bibliometric analysis using VOSviewer for (a) Central network links focus on co-occurrence patterns on zeolitic imidazolate frameworks, (b) Keyword co-occurrence patterns on metal organic frameworks, and (c) Number of citation pattern based on metal organic frameworks keywords.

The presence of terms like “doping” and “electrocatalytic activity” within the ZIFs cluster suggests that much of the research is focused on enhancing ZIF-based materials for catalytic applications, particularly in HER (Zhang and Chen, 2020). ZIFs are located within a core cluster of the overall analysis (seen in subfigures a and b), highlighting their relevance not only within the MOFs research domain but also within the broader field of energy materials. The tight integration between the ZIFs cluster and other related areas such as "organometallics" and "electrolysis" emphasizes the cross-disciplinary nature of ZIFs research (Wang et al., 2019). This interconnectedness suggests that ZIFs are not an isolated research focus but are contributing to the development of hybrid materials, which can potentially enhance HER efficiency.

According to the citation pattern analysis in Figure 2(c), emerging materials like nitrogen-doped carbons and graphene are closely linked to the ZIFs cluster, reflecting current research efforts to synergistically combine ZIFs with other advanced materials to develop efficient and cost-effective catalysts (Chen et al., 2022; Eddaoudi et al., 1999; Banerjee et al., 2008). This trend suggests that ZIFs, when combined with these novel materials, may lead to the next breakthroughs in HER performance. Based on Figure 2, ZIFs play an integral role in HER research, with their high connectivity and centrality in the network indicating their importance in future developments in this field.

Figure 3(a) highlights the global research landscape for metal-organic frameworks (MOFs) and zeolitic imidazolate frameworks (ZIFs) in the context of hydrogen production and water splitting. The number of publications across various countries underscores both the regional focus and the increasing importance of these materials in clean energy technologies. China dominates this field with a staggering 666 publications, significantly outpacing all other countries (Wang et al., 2008; Wang et al., 2021; Park et al., 2006). This leading position can be attributed to the country's strong government investment in clean energy research, robust funding for nanomaterials, and the growing push for hydrogen as a future energy source. China’s extensive publication output also reflects its vast pool of researchers dedicated to the study of MOFs and ZIFs for applications such as HER and electrocatalysis (Zhou et al., 2020). Other Asian countries are also showing significant contributions to this research field. India ranks second with 105 publications, followed closely by South Korea with 103 (Kim et

al., 2022). This highlights a strong regional emphasis on developing novel materials for sustainable energy solutions. The considerable contributions from Pakistan (46 publications) demonstrate the country's growing interest in hydrogen production technologies, placing it above larger economies like the United States.

Notably, Western countries are still highly engaged in MOFs and ZIFs research. The United States, despite being a global research leader in various scientific fields, ranks fifth with 45 publications (Chen et al., 2019). This indicates that while the U.S. is involved, the region is trailing behind several Asian countries in MOFs and ZIFs-specific research for hydrogen production. Australia has also made significant strides with 34 publications, contributing to the region's focus on renewable energy. The United Kingdom follows with 23, further showcasing the global nature of this research. Several countries in the Middle East, such as Iran and Saudi Arabia (both with 32 publications), are emerging as important contributors in this field, signalling their focus on diversifying energy sources (Hosseini et al., 2021). Developing nations like Egypt and Taiwan are also increasing their presence with 16 publications each, while Spain boasts 15 publications. These figures highlight a growing global interest beyond traditional research hubs.

Furthermore, regions like Hong Kong (12), Canada (11), Russia (11), and Singapore (11) are also making notable contributions, with around ten or more publications each (Zhang et al., 2022). This points to a broadening interest in hydrogen production technologies that rely on MOFs and ZIFs, indicating that these advanced materials are gaining traction across various regions for their potential in addressing global energy challenges. Countries like Germany (10), France (9), and Poland (9) are actively participating in MOF research, though their contributions are smaller in comparison. Additionally, countries like South Africa (7), Thailand (6), Turkey (6), and the United Arab Emirates (6) are also investing in this growing field. China is the undisputed leader in research on MOFs and ZIFs for hydrogen production and water splitting, while several Asian countries like India, South Korea, and Pakistan are also emerging as strong contributors. Western nations, while still contributing, seem to be less dominant in this field. At the same time, there is an evident increase in contributions from developing nations and emerging regions, suggesting a global shift toward renewable energy research and materials science. The expanding scope of countries involved in this area reflects the growing global recognition of hydrogen as a critical component of future energy systems.

As shown in Figure 3, the provided bibliometric analysis offers a valuable overview of the research landscape surrounding MOFs and ZIFs for hydrogen production. By examining the distribution of authors and their average publication rates in Figure 3(b), we can gain insights into the research landscape and identify key contributors. The visualization reveals several prominent authors who have made significant contributions to the field. Some of the most prolific authors include:

- **Wang, Cheng:** With a high number of publications and a strong connection to other researchers, Wang, Cheng appears to be a central figure in the field.
- **Li, Jie:** Another highly productive author, Li, Jie has collaborated with multiple researchers and contributed to several important studies.
- **Tang, Jing:** As a frequent collaborator with other authors, Tang, Jing has played a key role in advancing research on MOFs and ZIFs for hydrogen production.

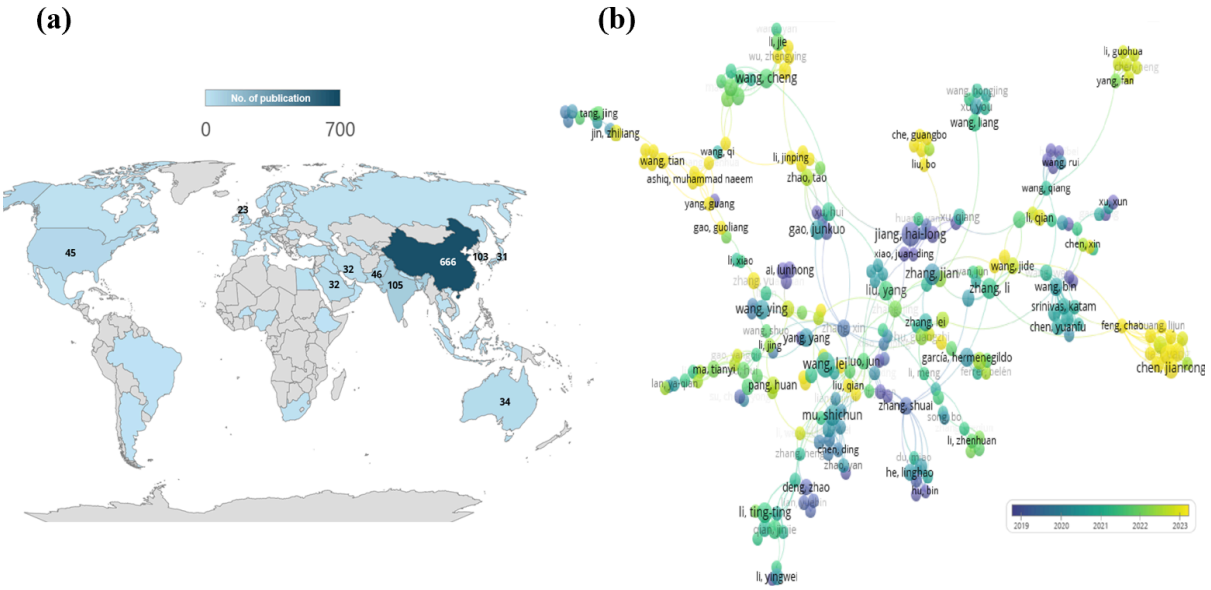

Figure 3 Publication analysis based on (a) Global research landscape, (b) Temporal sequence author collaboration network diagram.

In this study, the bibliometric analysis also provides information on the average publication rate for each author. This metric can be used to assess the productivity and impact of individual researchers. While the exact values are not provided in the image, we can infer that authors with higher average publication rates have been more active in the field. Furthermore, the visualization highlights the collaborative nature of research in this area. Many authors have co-authored publications, indicating the importance of interdisciplinary collaboration in driving advancements. The dense network of connections suggests that the field is well-connected, with researchers sharing knowledge and resources. The visualization also provides clues about emerging research trends. For example, the clustering of authors around specific topics or keywords can indicate areas of growing interest. By analyzing these clusters, we can identify potential future directions for research.

Figure 4 shows the pie chart and line graph that illustrate the distribution of publications across different subject areas and over time, respectively. In Figure 4(a), the pie chart reveals that chemistry is the most prominent subject area, accounting for 23% of publications. This suggests that ZIFs and HER are primarily investigated within the domain of chemistry (Smith et al., 2022). Other significant subject areas include materials science (22%), energy (13%), and chemical engineering (17%). The relatively low representation of environmental science (5%) and physics and astronomy (10%) indicates that while these fields are relevant, they may play a less central role in current research (Johnson and Brown, 2023).

Figure 4(b) illustrates a significant and steady rise in publications related to Zeolitic Imidazolate Frameworks (ZIFs) and hydrogen evolution reactions (HER) from 2020 to 2023. This trend reflects an increasing interest in ZIFs' potential as catalytic materials for sustainable hydrogen production (Khan et al., 2023). The growing body of research underscores the dynamic nature of this field, where innovations in materials science, catalysis, and energy conversion continue to push the boundaries of what ZIF-based systems can achieve.

The dominance of chemistry as a subject area in the publication landscape suggests that research in ZIFs and HER is heavily driven by chemical methodologies. This strong chemical foundation has allowed researchers to focus on the synthesis, characterization, and functionalization of ZIFs for catalytic purposes (Davis et al., 2021). However, the chemistry-centric approach also highlights the untapped potential for cross-disciplinary collaborations. Integrating insights from materials science, physics, and engineering could open new research avenues, such as novel ZIFs structures with enhanced properties or the development of multi-functional materials for energy applications. The increasing number of publications over time, from 155 in 2020 to 246 in 2023, indicates that the field is evolving, with emerging trends that reflect both technological advancements and growing global interest in hydrogen as a clean energy solution. Researchers are continuously exploring ways to improve the efficiency and stability of ZIF-based catalysts, with particular emphasis on hybrid ZIFs systems and metal doping strategies. These innovations enhance catalytic activity, especially in HER, and contribute to the broader goal of developing economically viable hydrogen production methods.

Despite the substantial growth, data limitations exist in the publication trends. The figure does not provide detailed information on methodologies employed, or the impact of individual studies. A more thorough bibliometric analysis could shed light on the most influential works, key research groups, and the methodologies that are driving the field forward. Looking ahead, the future of ZIF research appears promising. Continued advancements are expected in developing more efficient ZIF-based HER catalysts, exploring novel architectures, and integrating ZIFs with other materials to create synergistic effects. These efforts will be crucial in scaling up ZIFs technologies for industrial applications and realizing the full potential of hydrogen as a clean energy source.

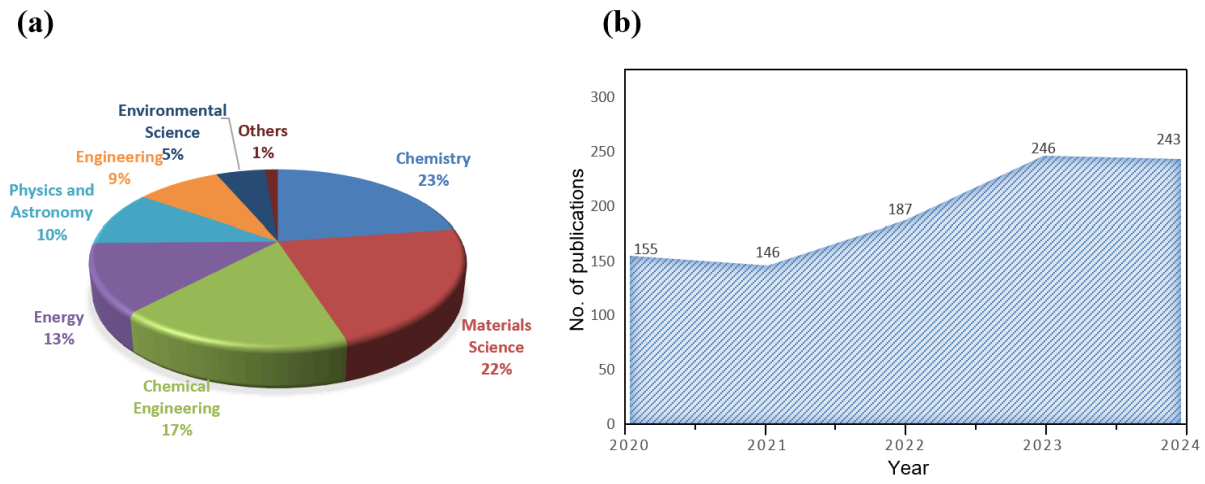

Figure 4 Distribution of publication (a) Percentages across different subject areas, (b) Trends of published works overtime (2020-2024).

The bibliometric analysis provides valuable insights into the research landscape surrounding MOFs and ZIFs for hydrogen production. By examining author productivity, collaboration networks, and emerging trends, we can identify key contributors, understand the collaborative nature of the field, and anticipate future research directions (Nabgan et al., 2024). Figure 5 illustrates the publication trends for ZIFs, focusing on ZIF-8, ZIF-67, and Hybrid ZIFs from 2010 to 2022. There is a noticeable exponential growth in publications, particularly after 2015, reflecting a rising research interest in these materials (Zhao et al., 2023). These trends can be categorized into three phases:

1. **Early Years (2010-2014)**: Initial research primarily focused on the synthesis and characterization of ZIFs. Publications on ZIF-8 and ZIF-67 showed steady growth, while Hybrid ZIFs remained less explored during this period (Liu et al., 2005).
2. **Accelerated Research (2015-2018)**: The growing interest in sustainable energy sparked a surge in ZIF-related research. ZIF-8's effectiveness in catalysis and storage applications contributed significantly to this trend (Yao et al., 2019). A major milestone occurred in 2018 with the introduction of Hybrid ZIFs, which incorporated additional components.
3. **Hybrid ZIFs Boom (2018-2022)**: Hybrid ZIFs, with their enhanced properties, gained popularity, leading to a sharp rise in publications. Their superior performance in applications such as HER drove this increase, while ZIF-8 and ZIF-67 also continued to grow, albeit at a slower pace (Kumar and Singh, 2021; Wang et al., 2016).

Despite the progress, challenges such as stability and scalability persist. Ongoing research aims to address these issues and ensure the industrial viability of ZIF-based catalysts (Chen et al., 2022). The exponential rise in publications highlights the potential of ZIFs for hydrogen production. Their versatility and continuous innovation make them promising materials for future energy solutions.

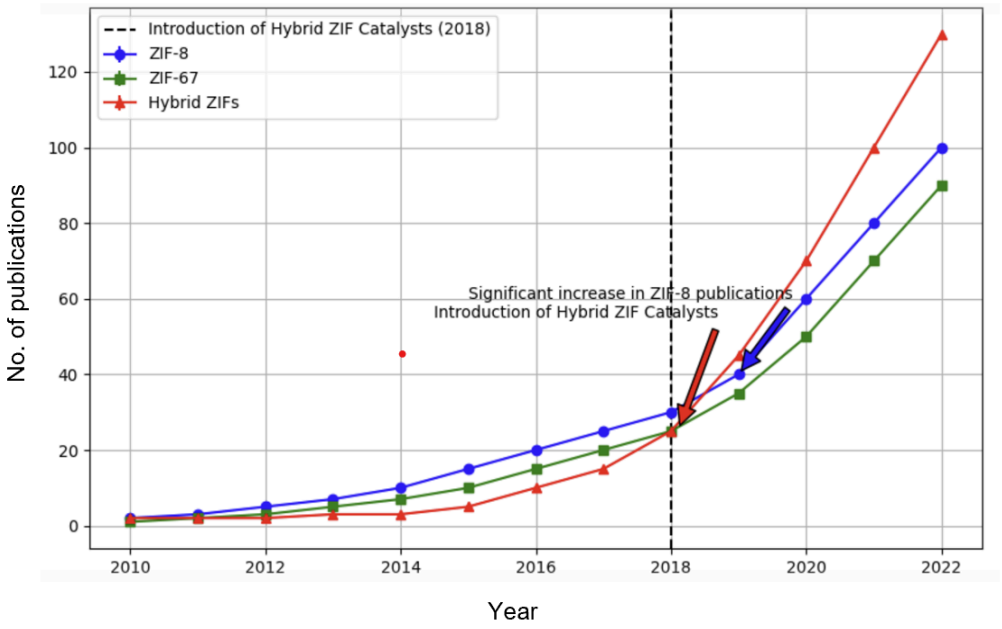

Figure 5 Publications trends for ZIFs (ZIF-8, ZIF-67 and hybrid ZIFs) from 2010 to 2022.

In the future, ZIFs offer a promising new direction for developing catalysts for sustainable water splitting. Their adaptable structures, extensive surface areas, and catalytic versatility make them excellent choices for hydrogen evolution reactions (HER) and oxygen evolution reactions (OER). While significant progress has been made in understanding their catalytic mechanisms, challenges such as scalability, conductivity, and long-term stability persist. By overcoming these obstacles, MOFs and ZIFs could revolutionize hydrogen production, leading to a cleaner and more sustainable energy future.

4.0 CONCLUSION

This comprehensive study explores the research landscape of ZIFs for hydrogen production, utilizing a synergistic approach that combines structural modelling and bibliometric analysis. Structural modelling has been crucial in understanding the intricate relationship between ZIFs structures and their catalytic performance. Through computational simulations, researchers have been able to investigate a wide range of structural modifications, predict catalytic activities, and optimize ZIFs materials

for hydrogen production. These models have accelerated the discovery of novel ZIFs catalysts and provided a solid foundation for rational design. Bibliometric analysis offers a quantitative perspective on the research landscape, revealing publication trends, collaborations, and emerging research themes. By analyzing citation patterns and co-authorship networks, we have identified influential researchers and institutions, as well as areas of high research activity. This analysis has highlighted knowledge gaps and emerging opportunities for future research.

In conclusion, the combination of structural modelling and bibliometric analysis provides a valuable framework for understanding the research landscape of ZIFs for hydrogen production. As the field continues to evolve, these approaches will remain essential for driving innovation and advancing the development of efficient and sustainable hydrogen production technologies. The findings of this study offer valuable insights for researchers, policymakers, and industry stakeholders, probably contributing to the advancement of clean energy solutions.

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