

Systematic Review

Performance Benchmarking of MOF-Based Adsorbents for Organic Dye Removal: A PRISMA-Guided Bibliometric and Statistical Analysis

Arely Montserrat Canton-Diaz, Juan Jose Alonso-Tijerina  and Nancy Elizabeth Davila-Guzman * 

Facultad de Ciencias Químicas, Universidad Autónoma de Nuevo León, Ciudad Universitaria, Av. Universidad s/n., Nuevo León 66455, Mexico; arely.cantondi@uanl.edu.mx (A.M.C.-D.); juan.alonsotjr@uanl.edu.mx (J.J.A.-T.)

* Correspondence: nancy.davilagz@uanl.edu.mx

Abstract

This study presents a PRISMA-guided bibliometric and statistical analysis of MOF-based adsorbents for organic dye removal, covering publications from 2014 to 2026. A total of 59 studies were analyzed to evaluate research trends, material classification, and adsorption performance under diverse experimental conditions. The results revealed clear differences in adsorption behavior depending on dye type, molecular properties, and operational conditions, highlighting the key role of electrostatic interactions and solution chemistry. From a materials perspective, pristine MOFs dominated the literature; however, a transition toward functionalized and composite materials was identified, driven by the need to improve adsorption efficiency, selectivity, and stability. MIL-, UiO-, and ZIF-type frameworks were the most frequently investigated due to their balance between structural stability and adsorption performance. The analysis also identified critical limitations, particularly the inconsistent reporting of key experimental parameters, which limits comparability and hinders the identification of reliable structure–property relationships. Overall, this study provides a benchmarking framework supporting the rational design of MOF-based adsorbents for wastewater treatment applications.

Keywords: metal–organic frameworks; MOF; dye; adsorption; bibliometric analysis; PRISMA

1. Introduction

Water pollution caused by organic dyes from textile, pharmaceutical, and chemical industries represents a major environmental challenge. These compounds are often persistent, toxic, and resistant to conventional treatment processes, posing significant risks to aquatic ecosystems and human health [1,2]. Among the available treatment technologies, adsorption has emerged as a promising approach due to its simplicity, efficiency, and potential for large-scale implementation [3]. In addition to MOF-based materials, increasing attention has been directed toward sustainable biomass-derived adsorbents and other environmentally friendly remediation strategies for wastewater treatment. Recent studies have explored the use of agricultural residues and waste-derived materials as low-cost adsorbents, highlighting their potential for pollutant removal and resource valorization [4–6]. In recent years, metal–organic frameworks (MOFs) [7] have attracted considerable attention as advanced adsorbents for dye removal [8–10]. Their exceptionally high surface area, tunable pore structures, and versatile chemical functionality enable selective adsorption and enhanced interaction with a wide range of organic contaminants.



Academic Editors: Anthony Harriman and Nadia Barbero

Received: 6 May 2026

Revised: 9 June 2026

Accepted: 19 June 2026

Published: 14 July 2026

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Numerous studies have reported high adsorption capacities for different types of dyes, including azo, anthraquinone, and xanthene, confirming the effectiveness of these materials in aqueous systems [11–13].

Despite the rapid growth of research in this field, significant challenges remain. Conventional adsorbents often exhibit limited selectivity, low regeneration capacity, and reduced performance under complex conditions such as real wastewater matrices [14,15]. Although MOF-based materials offer clear advantages, their performance is strongly influenced by structural properties, surface chemistry, and interactions with specific dye molecules [16–18]. While a large number of studies have investigated MOF-based adsorbents, the absence of a systematic benchmarking framework integrating structure–property relationships, normalized adsorption metrics, and performance under comparable experimental conditions represents a critical knowledge gap. Existing studies often report adsorption capacities under different experimental conditions, making direct comparison difficult and limiting the identification of optimal material design strategies [19]. This limitation is also evident in recent review articles, where differences in experimental conditions hinder direct benchmarking across materials. Several recent review articles have summarized advances in MOF-based materials for dye removal, including MOF composites, heteroatom-doped frameworks, environmental remediation applications, and specific MOF families such as MIL-, UiO-, and ZIF-based materials. These reviews have provided valuable insights into synthesis strategies, adsorption mechanisms, material modifications, and practical applications. However, they are primarily narrative in nature and generally do not incorporate a systematic PRISMA-guided selection methodology combined with bibliometric analysis and quantitative benchmarking of adsorption performance across different MOF families, dye classes, and operational conditions. Consequently, the identification of general performance trends and structure–property relationships remains challenging due to the heterogeneity of experimental conditions and reporting practices. To address this limitation, the present study applies predefined eligibility criteria to construct a standardized dataset and combines a PRISMA-guided systematic review with bibliometric and statistical analyses. This approach enables a more consistent comparison of adsorption performance and facilitates the identification of trends, relationships, and knowledge gaps within the current literature [20–25]. Therefore, the aim of this study is to conduct a PRISMA-guided systematic review, bibliometric, and statistical evaluation of MOF-based materials for organic dye removal. This work integrates material taxonomy, dye classification, molecular descriptors, and performance benchmarking to identify key trends, relationships, and limitations in the current literature [26,27]. By providing comprehensive and standardized analysis, this study contributes to the development of more efficient and scalable MOF-based adsorbents for wastewater treatment applications [28].

2. Materials and Methods

This study was conducted in accordance with the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA 2020) guidelines to ensure transparency and reproducibility during the identification, screening, and selection of relevant publications [29]. The methodology combined a PRISMA-guided systematic review with bibliometric and statistical analyses to evaluate publication trends, classify adsorbent materials and dye types, and compare adsorption performance reported in the literature [30]. A bibliometric–statistical analysis was conducted to evaluate scientific publications related to the adsorption of organic dyes using metal–organic frameworks (MOF). The literature search was performed on the Web of Science [31] which is widely recognized for its coverage of high-quality peer-reviewed scientific publications.

2.1. Literature and Search Strategy

For bibliometric and PRISMA analyses, the search strategy was developed using combinations of keywords related to MOFs materials and dye adsorption processes. The following search terms were included: “metal-organic framework” OR “MOF”, “dye adsorption” OR “organic dye removal”, “adsorption capacity”, “regeneration”, and “wastewater”. Boolean operators AND and OR were applied to refine the search queries and improve retrieval accuracy [32]. Only peer-reviewed journal articles written in English were considered eligible for inclusion. The search was limited to studies published between 2014 and 2025. The complete search strings, filters applied, and number of retrieved records are summarized in Table 1.

Table 1. Detailed search strategy applied in Web of Science (WoS), including keywords, Boolean operators, filters, and number of records retrieved.

Database	Search String (Keywords and Boolean Operators)	Filters Applied	Records Retrieved
Web of Science (WoS) Strategy 1	(“metal-organic framework*” OR MOF* OR ZIF* OR UiO* OR MIL* OR HKUST* OR PCN*) AND (dye* OR azo dye* OR anthraquinone dye* OR xanthene OR methylene blue OR rhodamine B OR congo red) AND (adsorption OR removal) AND (isotherm* OR kinetic* OR mechanism*) AND (column OR fixed bed OR breakthrough) AND (real wastewater OR effluent OR textile OR salinity OR NOM)	Articles; English; Science Citation Index Expanded; 2014–2025	1300

Note: * denotes the wildcard operator used in the Web of Science search strategy.

2.2. Identification and Screening

The study selection process followed the four-stage procedure recommended by PRISMA 2020, including identification, screening, eligibility, and inclusion of relevant studies [33,34]. Duplicate records were removed based on a comparison of titles and Digital Object Identifiers (DOI). Subsequently, titles and abstracts were screened to exclude studies not related to dye adsorption using MOF-based materials. The remaining articles were then subjected to full-text assessment according to the predefined inclusion and exclusion criteria. The complete workflow of the study selection process is illustrated in the PRISMA flow diagram (Figure S1) [34]. The final set of studies included in the bibliometric–statistical analysis was obtained after applying the selection criteria (Table S1).

2.3. Study Selection and Criteria

The eligibility criteria were defined prior to the screening process to ensure methodological consistency during study selection. The inclusion and exclusion criteria applied for article selection are summarized in Table S1.

Studies were selected based on predefined inclusion and exclusion criteria to ensure consistency across the dataset. Eligible studies focused on the adsorption of organic dyes in aqueous systems using MOF-based materials and reported quantitative adsorption data under clearly defined experimental conditions [35]. Only peer-reviewed journal articles published in English within the selected time frame were considered. Studies were excluded if they did not meet these requirements, including insufficient experimental detail, absence of adsorption capacity data, or focus on non-aqueous systems, non-MOF materials, or non-experimental approaches. Duplicate records and secondary sources were also removed. The selection process followed PRISMA guidelines, including an initial screening based on titles and abstracts, followed by a full-text review to determine eligibility [36]. The final set of selected studies was subsequently used for bibliometric and statistical analysis.

2.4. Data Extraction and Normalization

Data from the selected studies were systematically extracted following a predefined protocol to enable bibliometric and statistical analysis of MOF-based materials for dye adsorption. For each eligible article, the following variables were recorded: type of MOF material, surface area, pore volume, pore size; dye identity, including classification by charge (cationic/anionic) and chemical structure (e.g., azo, anthraquinone, xanthene), and maximum adsorption capacity ($q_{\max}$, mg g^{-1}), solution pH, temperature, regeneration cycles. These variables were selected to capture key information related to adsorbent characteristics, experimental conditions, and adsorption performance indicators reported in the literature.

To facilitate comparison between studies, maximum adsorption capacities obtained from Langmuir model were standardized to mg g^{-1} . When necessary, unit conversions were applied to ensure consistency across the compiled dataset. The extracted data were organized into a structured tabular database (Table S1), which served as the basis for subsequent statistical and comparative analyses aimed at identifying performance trends and relationships between MOF materials, dye properties, and operational conditions [37]. Only molecular descriptors consistently reported across studies, such as dye charge and class, were included in the comparative analysis, as the inconsistent reporting of other descriptors prevented their reliable inclusion. For anionic dyes, pK_a values, solution pH, and the point of zero charge (pH_{PZC}) of the adsorbent were collected whenever available in the original studies. These parameters were used to examine the possible role of electrostatic interactions in the adsorption process by comparing the reported pH values with the corresponding dye pK_a values and by evaluating $\Delta(\text{pH}-\text{pK}_a)$. Due to the limited availability and inconsistent reporting of pH_{PZC} data, the analysis was restricted to a qualitative interpretation of adsorption trends.

2.5. Statistical and Benchmarking Analysis

A comparative performance benchmarking analysis was conducted to evaluate the adsorption performance reported across the selected studies. The analysis focused on the following aspects: distribution of adsorption capacity across different MOF families, performance differences among dye classes, and regeneration stability trends. Descriptive statistical parameters, including mean, median, and range, were calculated to summarize the reported adsorption capacities. In addition, adsorption capacity normalized by BET surface area ($q_{\max}/S_{\text{BET}}$) was calculated for studies reporting both $q_{\max}$ and BET surface area values. This parameter was used as an exploratory metric to evaluate adsorption efficiency relative to the available surface area and to avoid overinterpreting BET surface area as the sole determinant of adsorption performance. Differences among pristine, functionalized, and composite MOFs were further examined using the non-parametric Kruskal–Wallis test. A non-parametric approach was selected because of the heterogeneity of the compiled dataset, including differences in dye type, adsorption conditions, and material characteristics. Statistical significance was evaluated at a confidence level of 95% ($p < 0.05$). The descriptive statistics and results of the exploratory Kruskal–Wallis analyses are provided in Tables S3 and S4 of the Supporting Information.

Additionally, an exploratory trend analysis was performed to identify potential relationships between MOF structural characteristics, dye molecular descriptors, and adsorption performance. The extracted data were compiled into comparative benchmark tables and evidence maps to highlight performance trends across MOF families and dye classes. Mechanistic interpretation was conducted by examining qualitative relationships between dye molecular descriptors and MOF structural features, including pore aperture, functional groups, and surface charge.

Additionally, the bibliometric analysis included the generation of a co-occurrence map of keywords (minimum frequency > 5), allowing the visualization of relationships between research topics [38]. The analysis also quantified the number of publications per year, identifying temporal trends, as well as the distribution of publications by country, MOF material, and dye class. Collaboration maps were generated to reveal networks of co-authorship and institutional cooperation, while term co-occurrence maps were used to explore the connections between important concepts across titles, abstracts, and keywords, highlighting emerging themes and relationships between research topics. The software used for the analyses was RStudio (Version 4.5.3) and Biblioshiny [37].

3. Results

3.1. Dataset Overview and Study Selection

A total of 59 documents published between 2014 and 2025 were analyzed, covering a wide range of scientific sources (43 journals). In terms of citation metrics, the dataset presents an average of 6.56 citations per document, with an overall average citation count of 96.81, reflecting moderate scientific impact across the selected studies. Regarding authorship, a total of 304 authors contributed to the dataset, with only 1 single-authored document, highlighting the strong prevalence of collaborative research. The average number of co-authors per document (5.54) further supports the presence of multi-author research networks, while an international co-authorship rate of 22.03% indicates a moderate level of global collaboration. Additionally, the dataset includes 225 Keywords Plus (ID) and 167 author keywords (DE), suggesting a diverse thematic coverage within the field.

The study selection process is summarized in Figure S1, following the PRISMA 2020 guidelines [33]. A total of 1737 records was identified using the primary search string in Web of Science. After applying the filters described in Table 1, a total of 437 records were excluded. The resulting records (1300) were screened based on titles and abstracts, resulting in the exclusion of 1172 records. Finally, an additional 79 records were excluded due to the inability to retrieve the full text. Based on this dataset, a bibliometric analysis was conducted using the 59 documents obtained from Web of Science. The selection process ensured a systematic and transparent identification of relevant studies.

3.2. Bibliometric Analysis

3.2.1. Publication Trends

The temporal distribution of publications related to the adsorption of organic dyes using metalorganic frameworks (MOF) is presented in Figure S2. A noticeable increase in research output can be observed starting from 2014, with a marked growth trend over the following years. Notably, 2020 stands out as the year with the highest number of publications, reflecting peak research interest in the topic [39]. However, it can be observed that research interest in adsorption persists in the subsequent years. It is important to note that the publications analyzed here correspond only to those that met the predefined inclusion criteria; therefore, this figure does not represent all available studies in the field.

The distribution of dyes investigated in the reviewed studies is shown in Figure 1. Methylene blue (MB) was the most frequently studied dye, with a total of 37 occurrences, followed by Congo red (CR) with 20, methyl orange (MO) with 8, and rhodamine B (RhB) with 7. Other dyes were reported with considerably lower frequencies, appearing only sporadically across the literature. In studies involving multiple dyes, each compound was considered independently to ensure an accurate representation of its frequency across the literature [40]. This distribution highlights a clear research focus on representative cationic and anionic dye systems. Methylene blue emerged as the most widely used model of dye, is likely due to its well-characterized properties, high solubility, and ease of detection

using spectrophotometric techniques [41]. Similarly, Congo red and methyl orange were frequently selected as representative anionic azo dyes, reflecting the growing interest in evaluating adsorption performance toward negatively charged contaminants [42]. Overall, these findings suggest that studies tended to prioritize model dyes with well-documented environmental relevance and distinct molecular structures, facilitating comparison across different MOF-based materials and experimental conditions [43]. This distribution also suggests a systematic preference for a limited set of model dyes, which, while enabling comparison across studies, may restrict the evaluation of MOF performance under more complex and realistic environmental conditions.

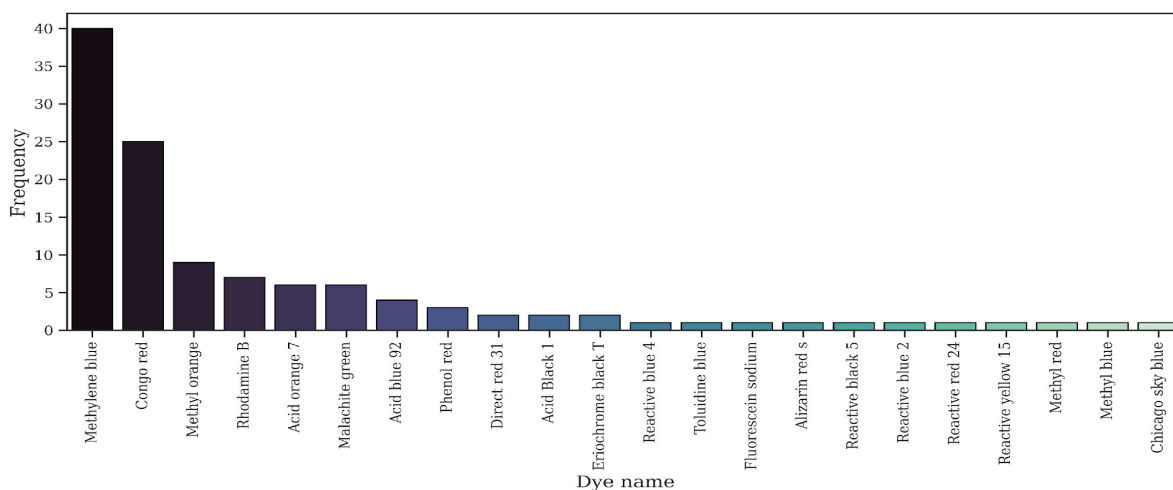


Figure 1. Distribution of dyes investigated in the analyzed literature.

3.2.2. Keyword Co-Occurrence Analysis

The keyword co-occurrence network shown in Figure 2 provides insight into the conceptual structure of the field. The analysis revealed that the most frequently used keywords were related to adsorption, removal, metal-organic frameworks, and methylene blue, indicating the main research focus. Several clusters were identified within the network, representing distinct but interconnected research themes. These included adsorption mechanisms, the development of MOF-based materials, and environmental remediation applications [44]. The strong connections between these keywords suggested that material design and adsorption performance were closely linked, forming the core of current research efforts.

3.2.3. Collaboration Networks

The collaboration network among countries and authors is shown in Figure 3. The network exhibits several distinct clusters, indicating that research activity is organized into interconnected groups. These clusters suggest that collaborations are often influenced by geographical proximity, institutional partnerships, and regional research frameworks. Inter-cluster connections are also observed, reflecting the presence of international collaborations that enable knowledge exchange across different regions. Overall, the network shows a moderate level of connectivity, suggesting that global integration in this field remains limited.

The distribution of scientific production by country (Figure 3) revealed a clear predominance of China, followed by Iran and India. Other countries, including South Korea, the United States, and Malaysia, contributed with comparatively lower publication output. This pattern indicates a strong regional concentration of research activity, particularly in Asia. Highly connected nodes within the network correspond to key authors and institu-

tions, highlighting their role in shaping research directions and facilitating collaboration in MOF-based adsorption studies.

The temporal evolution of scientific production in this field is presented in Figure S2 (Supplementary Materials), illustrating the sustained growth of research on MOF-based adsorbents for organic dye removal over the analyzed period.

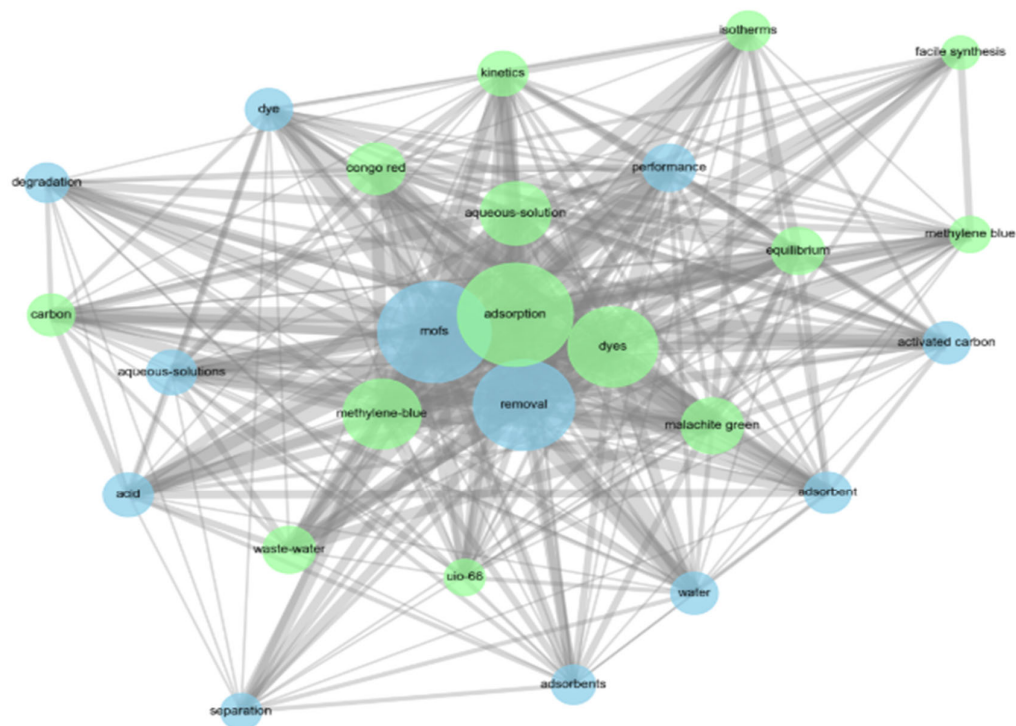


Figure 2. Keyword co-occurrence network showing the main research clusters.

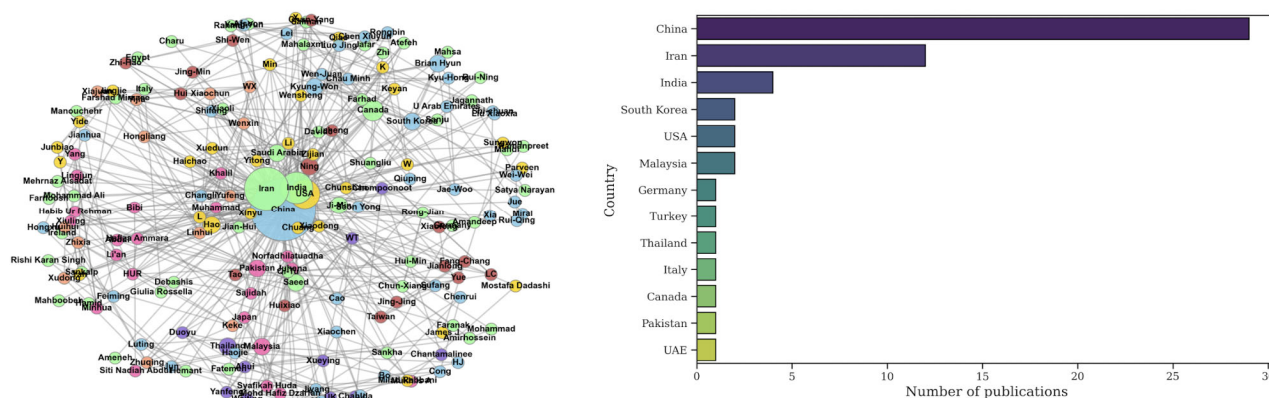


Figure 3. Global scientific production by country (left) and scientific production by country based on the number of publications (right).

3.3. MOF Classification and Structural Design Trends

3.3.1. MOF Classes

The distribution of material types in the analyzed dataset was presented in Figure 4. Metal–organic framework (MOF) adsorbents reported in the selected studies were classified into three main categories: pristine, functionalized, and composites. Pristine MOFs included unmodified frameworks, while functionalized MOFs refer to frameworks modified with specific functional groups to enhance adsorption performance, selectivity, or chemical stability. In contrast, MOF-based composites correspond to hybrid materials obtained

by integrating MOFs with additional components such as polymers, carbon materials, or inorganic supports, improving mechanical stability, dispersion, and adsorption efficiency.

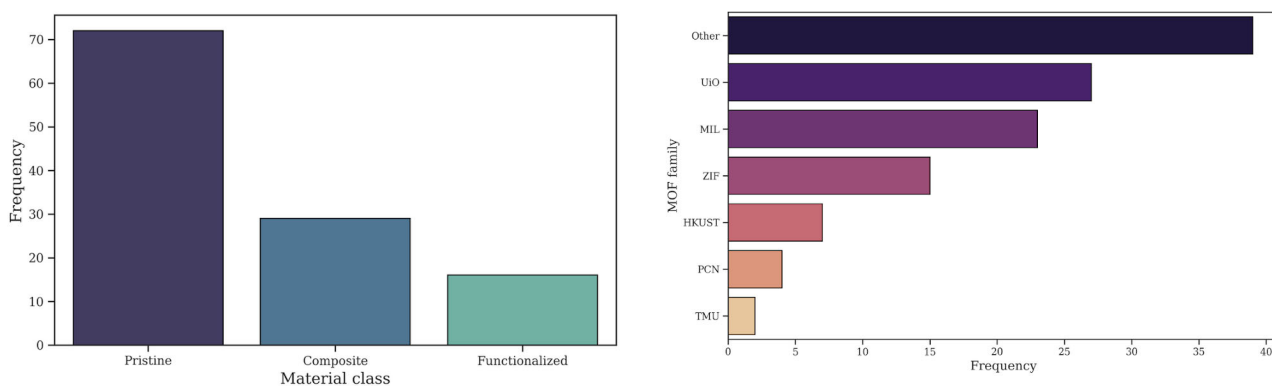


Figure 4. Quantitative distribution of MOF-based materials by classification category (**left**). Distribution of MOF families investigated in dye adsorption studies (**right**).

Using the classification criteria described above, the prevalence of each material class was quantitatively evaluated. Pristine MOFs constituted the largest proportion of the dataset ($n = 71$; 62.28%), followed by MOF-based composites ($n = 29$; 25.44%) and functionalized MOFs ($n = 14$; 12.28%). The predominance of pristine MOFs indicated that research efforts were largely focused on fundamental framework structures. This trend was likely associated with their relatively straightforward synthesis, reproducibility, and well-established physicochemical properties which made them suitable model systems for understanding adsorption mechanisms. However, despite their prevalence, pristine MOFs often exhibited limitations in terms of stability under realistic aqueous conditions, selectivity toward specific pollutants, and reusability, particularly in complex matrices.

In contrast, the significant presence of composite and functionalized materials indicated a clear shift toward improving adsorption performance, selectivity, and stability. In particular, MOF-based composites integrated secondary materials such as magnetic nanoparticles, carbon-based supports, or polymers, which enhanced structural stability, facilitated separation and recovery, and improved dispersion in aqueous media. These features were especially relevant under non-ideal conditions, including emulsions, saline environments, or multicomponent systems.

Functionalized MOFs, although less frequently reported, represented a key strategy for tailoring adsorption behavior at the molecular level. The incorporation of functional groups (e.g., $-\text{NH}_2$, $-\text{COOH}$, or protonated sites) modified surface charge and pore environment, thereby strengthening electrostatic interactions and π - π interactions with dye molecules. This was particularly important for enhancing selectivity toward anionic dyes under controlled pH conditions.

Overall, the distribution of material class highlighted a transition from conventional pristine frameworks toward more complex and application-oriented materials, reflecting the increasing emphasis on practical performance and environmental applicability.

3.3.2. MOF Families

MOF families were classified as ZIF [45], UiO [46], MIL [47], PCN [10], TMU [48], and HKUST [49], since these materials have been widely investigated. Based on the 59 selected articles, a total of 117 MOF-family records were identified, as several studies reported more than one framework type. The “Other” category accounted for the highest proportion ($n = 39$; 33.33%), reflecting the presence of less frequently reported or non-standardized MOF structures. Among well-defined MOF families, UiO-based materials

represented the largest proportion ($n = 27$; 23.08%), followed by MIL-type structures ($n = 23$; 19.66%) and ZIF-based materials ($n = 15$; 12.82%). HKUST ($n = 7$; 5.98%), PCN ($n = 4$; 3.42%), and TMU ($n = 2$; 1.71%) were less frequently investigated (Figure 4). The predominance of UiO-based materials was attributed to their exceptional chemical and thermal stability, particularly under aqueous and acidic conditions, making them highly suitable for wastewater treatment applications. MIL-based materials were extensively studied due to their wide structural versatility and high stability, which allowed the incorporation of different metal nodes (e.g., Fe, Cr, Al) and organic linkers, enabling the tuning of pore size, surface chemistry, and adsorption sites. This versatility facilitated the design of materials tailored for specific dye adsorbent interactions, particularly through electrostatic attraction, π - π interactions, and hydrogen bonding. Similarly, ZIF structures were frequently reported because of their facile synthesis, high surface area, and good stability across a wide range of conditions.

In contrast, MOF families such as TMU and PCN were less frequently investigated, which may be attributed to their more complex synthesis routes, lower commercial availability, and in some cases, limited stability under aqueous or chemically harsh conditions.

Additionally, fewer studies have systematically evaluated their adsorption performance compared to more established frameworks such as UiO, MIL, and ZIF. A considerable number of materials were also reported using non-specific nomenclature (e.g., Fe-MOF, Cu-MOF, or Zr-MOF), highlighting a lack of standardization across the literature. Although this reflects the high structural diversity of MOF it may hinder direct comparison between studies and limit the development of unified design strategies. Overall, these findings indicate that research efforts have primarily focused on MOF families that offer a balance between stability, tunability, and adsorption performance, while also emphasizing the need for more consistent reporting practices.

3.3.3. Ligands

The distribution of primary ligands was analyzed based on the analysis revealed a clear predominance of carboxylate-based aromatic linkers, particularly terephthalic acid (BDC) and trimesic acid (BTC), reflecting the extensive use of well-established MOF structures such as UiO-66 and HKUST-1. This trend suggested that adsorption performance was largely investigated within a limited chemical space, where π - π interactions and structural stability were favored. In contrast, the low occurrence of functionalized and non-conventional ligands indicated that ligand engineering remained an underexplored strategy, despite its potential to enhance adsorption efficiency and selectivity, thereby emerging as a promising avenue for future research in the rational design of MOFs (Figure 5).

3.3.4. Metal Nodes

The frequency distribution of metal nodes identified in the analyzed studies is presented in Figure S3 (Supplementary Materials) and revealed a clear predominance of Zr-based frameworks, followed by Zn and Fe. Although this tendency could have been interpreted as an indication of superior performance, it was more accurately associated with a strong research preference for highly stable and well-established MOF families, particularly UiO-type structures. The widespread use of Zr was mainly attributed to its remarkable chemical and thermal stability, which made it especially suitable for dye removal in aqueous environments. Nevertheless, this imbalance also indicated a limited exploration of alternative metal centers, which may have restricted the diversity of adsorption mechanisms reported. Metals such as Ni, Ce, Ti, La, and Ag, which appeared less frequently, represented underexplored opportunities that could promote new interactions and potentially enhance adsorption efficiency. Despite their potential advantages, the

limited representation of metals such as Ti, Ce, and La may also be associated with practical considerations beyond adsorption performance. In some cases, precursor availability and synthesis costs are higher than those of more established metal nodes such as Zr, Zn, or Fe. Additionally, the synthesis of these frameworks may require more complex procedures, which can hinder scalability and large-scale implementation. Furthermore, information regarding their long-term stability under realistic wastewater conditions, including the presence of competing ions and complex matrices, remains comparatively scarce. These factors may partially explain their lower representation in the current literature despite their promising adsorption properties. From a structure-property standpoint, the selection of the metal node played a decisive role in adsorption behavior, as it influenced the coordination environment, surface characteristics, and the availability of active sites. These features governed key interactions, including electrostatic forces, coordination effects, and π - π interactions between the adsorbent and dye molecules.

Furthermore, the predominance of Zr-based materials may have introduced bias in performance comparisons, since most evaluations were conducted within a relatively narrow group of structurally similar systems. This constraint suggested that the current understanding of adsorption efficiency might not fully reflect the capabilities of less conventional MOF compositions. Overall, the observed distribution highlighted the importance of expanding the range of metal nodes explored in MOF design, particularly for the development of advanced adsorbents with improved functionality and applicability in complex aqueous systems.

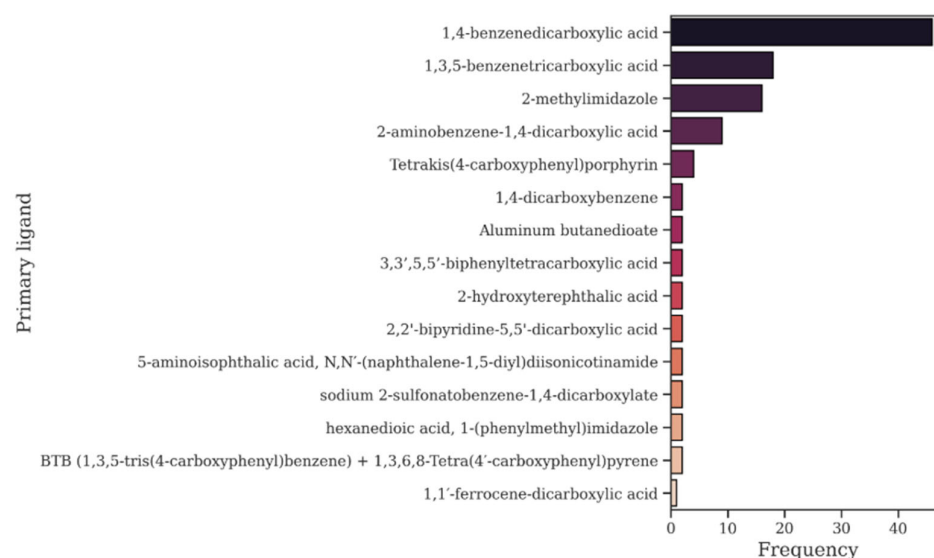


Figure 5. Frequency distribution of primary ligands used in MOF-based adsorbents for organic dye removal.

3.4. Operating Conditions and Experimental Variability

3.4.1. pH

The distribution of MOF families across different pH ranges (Figure 6) showed that UiO-based frameworks were predominantly employed under neutral conditions, while MIL and PCN structures exhibited a higher contribution in basic environments, and ZIF-based materials were consistently present across all pH ranges. In contrast, the distribution of dye classes revealed that azo dyes dominated under alkaline conditions, whereas thiazine dyes were more evenly distributed but remained prevalent under neutral conditions. These trends were consistent with the underlying adsorption mechanisms, where electrostatic interactions and π - π stacking played a key role. In alkaline conditions, the enhanced re-

removal of azo dyes may be associated with reduced competition from protons and stronger interactions with the adsorbent surface, while thiazine dyes, such as methylene blue, showed stable adsorption behavior across a broader pH range due to their cationic nature and affinity for aromatic frameworks. Overall, these observations suggest that both material selection and experimental conditions were closely aligned with the dominant adsorption mechanisms, potentially reflecting a bias toward optimized rather than realistic environmental scenarios.

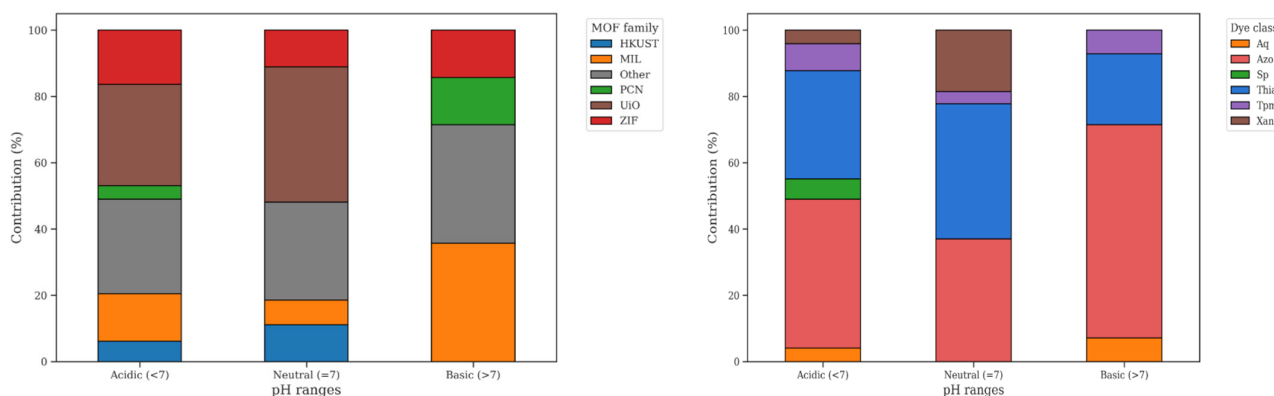


Figure 6. Contribution across different pH ranges (acidic, neutral, and basic) in dye adsorption studies: MOF families (left) and dye class (right).

3.4.2. Reusability

With respect to regeneration strategies and reusability cycles, the analyzed studies showed that regeneration was predominantly based on simple solvent washing, particularly using ethanol or methanol, whereas fewer studies employed chemical desorption or combined regeneration approaches. Notably, a considerable proportion of the literature did not explicitly report regeneration conditions, highlighting a lack of standardization in the evaluation of adsorbent reusability. Furthermore, the distribution of regeneration cycles showed that most studies assessed reusability within a limited range of 3–5 cycles, with a pronounced peak at four cycles. Beyond this range, the frequency of reported studies decreased markedly, indicating that long-term stability assessments remain insufficiently explored. The detailed distribution of regeneration cycles reported in the analyzed studies is presented in Figure S4 (Supplementary Materials). To further explore the role of dye speciation, the difference between experimental pH and dye pKa, denoted as $\Delta(\text{pH-pKa})$, was examined for anionic dyes using the data compiled in Table S2. A qualitative trend was observed in which the highest adsorption capacities (approximately $800\text{--}1315\text{ mg g}^{-1}$) were predominantly reported under conditions where pH was lower than the corresponding dye pKa, negative $\Delta(\text{pH-pKa})$ values. Under these conditions, the dye molecules are expected to be less ionized, which may reduce electrostatic repulsion and promote additional adsorption mechanisms such as hydrogen bonding, $\pi\text{-}\pi$ interactions, and enhanced pore accessibility. In contrast, lower and intermediate adsorption capacities were frequently observed at positive $\Delta(\text{pH-pKa})$ values. Although this trend suggests that dye speciation may influence adsorption performance, adsorption capacity cannot be explained solely by pH-dependent ionization, as framework topology, pore accessibility, surface chemistry, and specific adsorbent-adsorbate interactions also play important roles.

3.5. Adsorption Performance Benchmarking

The benchmarking of adsorption performance, expressed in terms of maximum adsorption capacity (q_{max}), demonstrates that the performance of MOF materials cannot be explained by a single dominant parameter. Instead, it results from a complex interplay

between structural features, textural properties, surface chemistry, operating conditions, and the physicochemical characteristics of the dye.

3.5.1. Dye Charge

Figure 7 shows how the maximum adsorption capacity varies with dye charge, distinguishing between anionic and cationic dyes. Overall, higher $q_{\max}$ values were observed for anionic dyes, both in terms of the median and the upper range of the data. The results for anionic dyes were also more spread out, with several values above 800 mg/g and some approaching 1200 mg/g. This suggested that, under certain conditions, MOFs can perform particularly well for these compounds. One possible explanation lies in the interactions between the dye molecules and the MOF surface. In many cases, MOFs provide active sites or functional groups that favor the adsorption of negatively charged species, for example through electrostatic attraction with metal centers or regions of partial positive charge. By contrast, cationic dyes may experience less favorable interactions, or even repulsion, depending on the surface chemistry of the material. The influence of dye charge should also be interpreted together with solution pH, as pH affects both dye speciation and the surface charge of MOF materials. Based on the experimental conditions compiled in Table S2, adsorption studies involving anionic dyes were conducted across a wide pH range, although many of the highest adsorption capacities were reported under near-neutral to moderately alkaline conditions. Under such conditions, electrostatic interactions may be enhanced through favorable surface charge development and reduced competition from protons. Nevertheless, the relationship between dye charge and adsorption performance cannot be attributed solely to pH, as adsorption behavior is also strongly influenced by MOF composition, functional groups, pore structure, and specific dye–adsorbent interactions. Therefore, the observed differences between anionic and cationic dyes likely arise from the combined effects of electrostatic interactions, framework chemistry, and experimental conditions. This interpretation is consistent with the pH-dependent adsorption conditions summarized in Table S2.

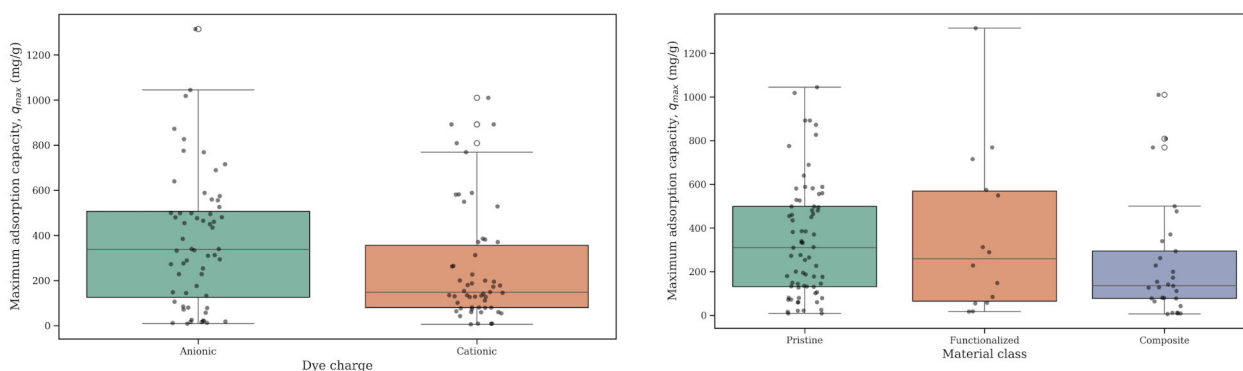


Figure 7. Maximum adsorption capacity for the organic dye removal as a function of dye charge (**left**) and material class (**right**). Grey, semi-transparent circles represent every individual, raw data point from the extracted dataset. White (or hollow) circles represent the statistical outliers (liers) calculated by the standard boxplot algorithm.

3.5.2. MOF Class

Several studies have explored the functionalization of MOFs as a strategy to improve adsorption performance. As shown in Figure 7, functionalized materials tended to exhibit higher $q_{\max}$ values within the analyzed dataset; however, direct statistical comparison was limited by the substantial heterogeneity of the experimental conditions reported across studies, including differences in dye type, pH, temperature, and adsorbent composition. To assess whether this pattern was statistically supported, an exploratory Kruskal–Wallis analy-

sis was performed using both $q_{\max}$ and $q_{\max}/S_{\text{BET}}$ values. The resulting p -values (0.058 and 0.212, respectively) indicated that differences among pristine, functionalized, and composite MOFs were not statistically significant at the 95% confidence level. Detailed descriptive statistics and test results are provided in Tables S3 and S4 of the Supporting Information. Therefore, although functionalized materials frequently exhibited higher adsorption capacities, the available dataset does not support a statistically significant advantage over the other material classes. This behavior was particularly evident for azo dyes, where functionalized materials often exhibited higher adsorption capacities than pristine counterparts. This improvement is likely related to the introduction of functional groups that increase the affinity between the adsorbent and the adsorbate, mainly through electrostatic interactions, hydrogen bonding, and π - π interactions. In contrast, composite materials do not consistently show better performance. In some cases, adding a secondary phase may even have a negative effect, for example by partially blocking the pores or reducing the accessible surface area. It is worth noting that many of these composites are prepared not only to enhance adsorption, but also to improve the handling and practical use of MOF powders in adsorption systems. This improvement is likely related to the introduction of functional groups that increase the affinity between the adsorbent and the adsorbate, mainly through electrostatic interactions, hydrogen bonding, and π - π interactions. In contrast, composite materials do not consistently show better performance. In some cases, adding a secondary phase may even have a negative effect, for example by partially blocking the pores or reducing the accessible surface area. It is worth noting that many of these composites are prepared not only to enhance adsorption, but also to improve the handling and practical use of MOF powders in adsorption systems.

3.5.3. MOF Family

Regarding the MOF family (e.g., ZIF, MIL, UiO, HKUST, TMU, PCN), a trend was observed that depends on the dye class (Figure 8). For azo dyes, UiO and MIL materials consistently showed higher $q_{\max}$ values, with several studies reporting capacities above 1000 mg/g. This behavior can be associated with their high chemical stability in aqueous media and the ease with which functional groups can be incorporated into their organic linkers, enhancing interactions such as π - π stacking, hydrogen bonding, and electrostatic attraction. In contrast, ZIFs displayed a wider variability in $q_{\max}$, suggesting that while some materials achieve high performance, the results are not consistent within this family. For thiazine dyes, PCN materials showed the highest average $q_{\max}$, followed by MIL and UiO, highlighting that topology and coordination chemistry influence adsorption differently depending on the dye.

An exceptionally high adsorption capacity ($q_{\max} = 6004.94 \text{ mg g}^{-1}$) was identified for a cotton blue-modified ZIF-67 system. According to the original publication, the enhanced adsorption performance was attributed to a synergistic adsorption mechanism in which pre-adsorbed sulfonated dye molecules generated additional interaction sites for methylene blue adsorption. Although this value was retained in the dataset because it met the predefined inclusion criteria, it represents a highly specific adsorption system and should not be considered representative of the overall performance of ZIF-based adsorbents.

3.5.4. Metallic Node

The maximum adsorption capacity across MOFs with different metal nodes is shown in Figure 8. A clear variability can be observed, suggesting that the choice of metal plays an important, although not exclusive, role in adsorption performance. MOFs built from Ti, Ce, and Zr tend to reach higher $q_{\max}$ values. In particular, Ti-based materials cover a wide range, with some cases approaching 1200 mg/g. This indicates that these systems

can perform very well, although not uniformly across all studies. Ce- and Zr-based MOFs show a similar tendency, with relatively high average values, which may be related to their structural robustness and the favorable surface chemistry they often provide for dye interaction.

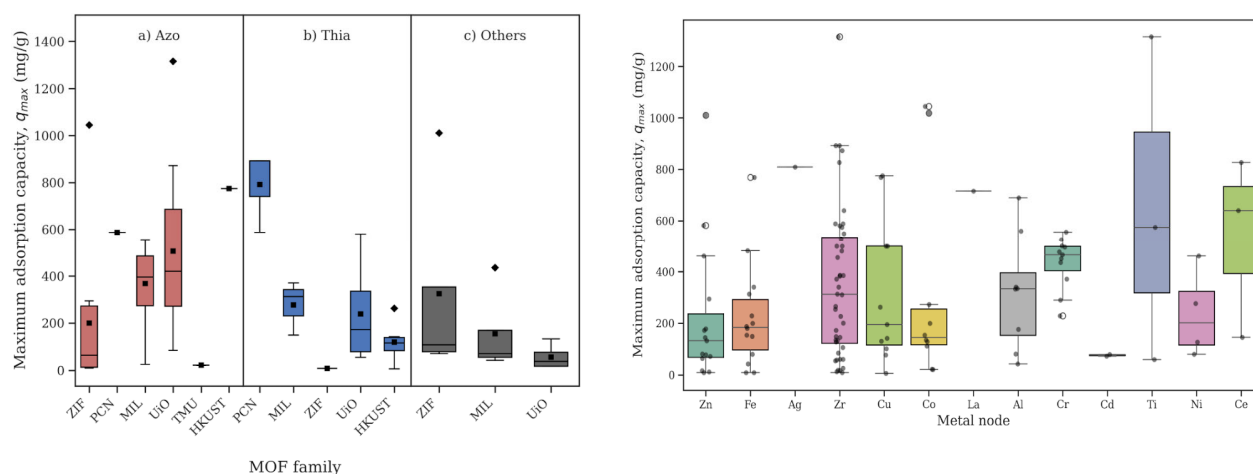


Figure 8. Distribution of maximum adsorption capacity ($q_{\max}$, mg g^{-1}) across different MOF families grouped by dye class (left) and metal node (right). The figure highlights the substantial variability in adsorption performance among different MOF families and metal nodes. Solid black squares indicate the arithmetic mean (average) of the distribution for that specific category. Solid black diamonds explicitly represent the statistical outliers (liers) falling outside the 1.5 IQR threshold. Grey, semi-transparent circles represent every individual, raw data point from the extracted dataset. White (or hollow) circles represent the statistical outliers (liers) calculated by the standard boxplot algorithm.

In contrast, materials containing Zn, Fe, or Co usually fall within a more moderate range of adsorption capacity. Their results are less scattered, which may reflect a more predictable but somewhat limited performance. For some metals, such as Cd, the distribution is both narrow and shifted toward low $q_{\max}$ values, which may reflect inherent limitations in adsorption performance or simply the smaller number of studies available for these systems. For Cu- and Al-based MOFs, the results appear more scattered. Some studies report relatively high capacities, but the overall distribution is quite uneven, suggesting that the outcome depends strongly on how the material is prepared and tested. On the other hand, Cr-based MOFs tend to show relatively high values with less variability, which could indicate a more stable adsorption behavior. Overall, while the metal node clearly matters, these results also make it evident that it cannot be considered in isolation, as its effect is closely linked to other characteristics of the material and the experimental conditions used.

3.5.5. Textural Properties

When looking at textural properties, particularly surface area, only a partial relationship with $q_{\max}$ was observed (Figure 9). While the highest adsorption capacities were generally reported for MOFs with surface areas above $1500 \text{ m}^2/\text{g}$, there is a noticeable spread in the data within each range. This suggests that surface area alone does not control the adsorption performance. In fact, some materials with intermediate surface areas ($500\text{--}1500 \text{ m}^2/\text{g}$) reach similar or even higher $q_{\max}$ values. This points to the importance of other factors, such as how accessible the pores are and how the active sites are distributed within the structure.

These results also highlight a common limitation in the literature, where surface area is often used as the main indicator of adsorption performance without considering whether that area is actually accessible to the adsorbate, particularly in relation to its molecular

size. As a result, the relationship between surface area and adsorption capacity should be interpreted with caution, especially in systems where diffusion limitations may play an important role.

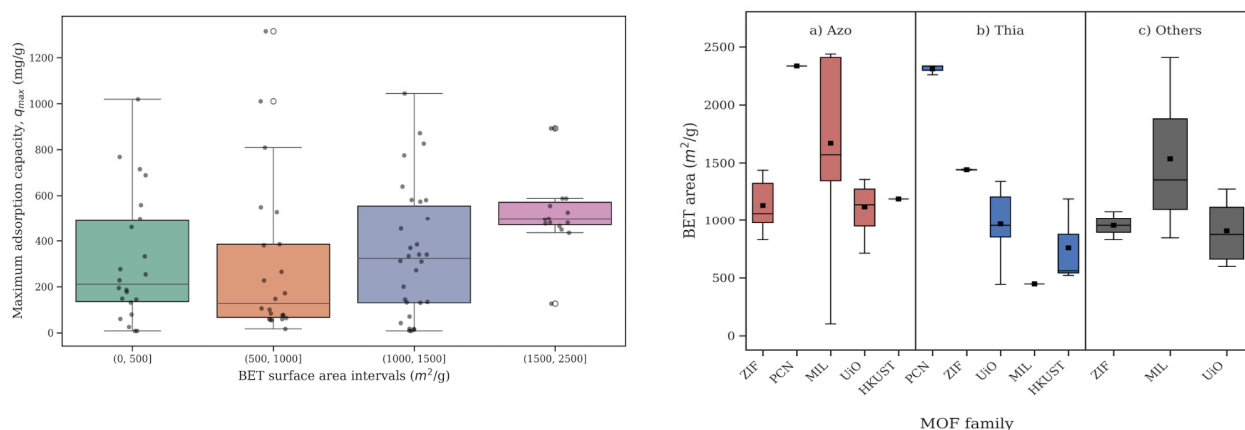


Figure 9. Distribution of maximum adsorption capacity ($q_{\max}$, mg g^{-1}) as a function of surface area (left) and distribution of BET surface area ($\text{m}^2 \text{g}^{-1}$) across different MOF families grouped by dye class (azo, thiazine, and others), highlighting the variability in textural properties among the analyzed materials (right). The figure illustrates the variability in both adsorption capacity and textural properties among the analyzed materials. Solid black squares indicate the arithmetic mean (average) of the distribution for that specific category. Grey, semi-transparent circles represent every individual, raw data point from the extracted dataset. White (or hollow) circles represent the statistical outliers (fliers) calculated by the standard boxplot algorithm.

An important distinction should also be made between total BET surface area and accessible surface area. While BET measurements provide an estimate of the overall porous surface available within a material, not all of this surface may be accessible to dye molecules under adsorption conditions. BET surface area is typically determined using N_2 adsorption at 77 K and therefore reflects the accessibility of a small gas probe under dry conditions. In contrast, dye molecules in aqueous solution are generally larger and surrounded by a hydration shell, which increases their effective size and may hinder diffusion through narrow pore apertures. Consequently, pore accessibility and pore connectivity can become more important than the total measured surface area, particularly for bulky dyes, where steric effects may restrict access to internal adsorption sites. To further explore this relationship, adsorption capacity was qualitatively normalized by BET surface area using the $q_{\max}/S_{\text{BET}}$ ratio. The calculated values covered a broad range ($0.006\text{--}127.55 \text{ mg m}^{-2}$), indicating considerable variability in adsorption efficiency among the analyzed materials. In several cases, materials with relatively moderate BET surface areas exhibited higher $q_{\max}/S_{\text{BET}}$ values than materials with substantially larger surface areas. These results indicate that adsorption performance cannot be predicted solely from BET surface area and that factors such as pore accessibility, framework topology, surface chemistry, and specific dye-adsorbent interactions also play an important role in determining adsorption efficiency.

The analysis of pore size offers a more detailed view of this relationship (Figure 10). For azo dyes, mesoporous materials (pore size $> 2 \text{ nm}$) generally show higher $q_{\max}$ values, likely because diffusion limitations are reduced and the molecules can more easily reach the active sites. However, this trend is not always observed. For thiazine dyes and other smaller or differently shaped molecules, both microporous and mesoporous materials can perform well. This suggests that adsorption is not controlled only by pore size, and that interactions between the dye and the MOF surface also play an important role. For this reason, the optimal pore size should not be treated as a fixed value, but rather as something

that depends on the specific adsorbate-adsorbent system. This point is especially important for the design of new materials. Instead of simply aiming for larger pores, it seems more effective to match the pore size to the size and shape of the target contaminant, so that access and interaction within the structure are not limited.

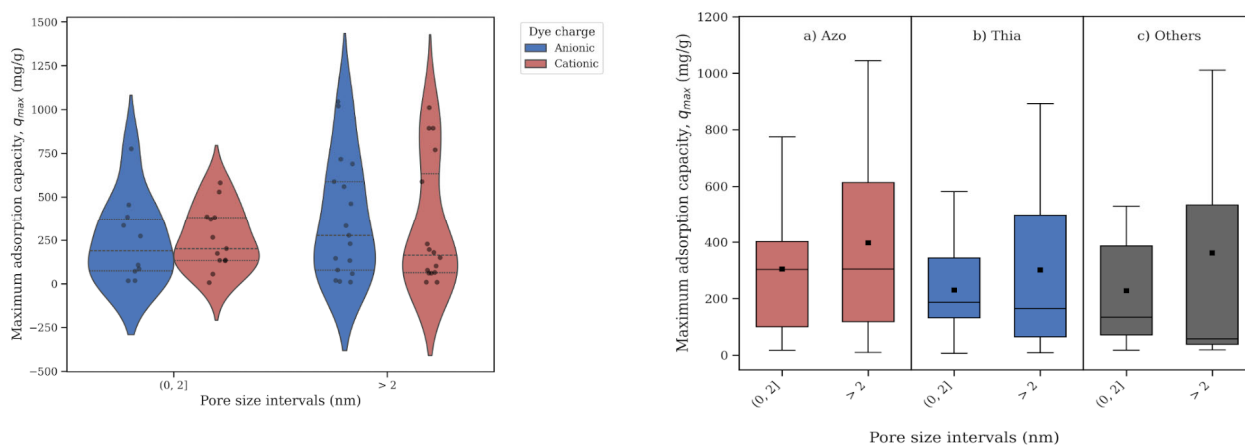


Figure 10. Violin plot of maximum adsorption capacity ($q_{\max}$, mg g^{-1}) as a function of pore size intervals ($(0, 2]$ and >2 nm), classified by dye charge (**left**) and dye class (**right**). The distributions illustrate the variability in adsorption performance across pore size ranges and dye categories. Black circles represent individual data points in the violin plots, and black squares indicate the mean values in the box plots. Solid black squares indicate the arithmetic mean (average) of the distribution for that specific category. Grey, semi-transparent circles represent every individual, raw data point from the extracted dataset.

3.5.6. Operating Conditions

Figure 11 illustrates the effect of two key operating variables, pH and temperature, on the maximum adsorption capacity. In both cases, a noticeable spread in the data can be observed, suggesting that these variables do not act independently but rather interact with other factors within the system. For pH, higher $q_{\max}$ values were generally observed under basic conditions ($\text{pH} > 7$) compared to acidic ones, especially for azo dyes. This trend may be related to changes in the ionization state of both the dye and the MOF surface, which can promote more favorable electrostatic interactions. Under neutral conditions, the results were more scattered, suggesting that more than one adsorption mechanism may be involved, including non-electrostatic interactions such as π - π interactions and hydrogen bonding.

The effect of temperature on $q_{\max}$ was examined over a range of 20 to 65 °C in the selected studies. However, most of the data (more than 90%) fall within a narrower interval, between 20 and 35 °C. In a few cases, temperature was varied mainly to perform thermodynamic analysis or to explore possible adsorption mechanisms, so those results were not considered here since they are not directly comparable. As shown in Figure 11, the intermediate range (26–35 °C) generally showed lower $q_{\max}$ values, with less variation between studies. By contrast, room temperature was the most commonly used condition for adsorption equilibrium experiments, and it is also where many of the higher $q_{\max}$ values were reported.

Taken together, these results suggest that pH tends to have a clearer influence on adsorption performance, while the role of temperature is still not well established. The wide spread of values in both cases also points to the fact that $q_{\max}$ depends on several factors at the same time, including the type of MOF, the nature of the dye, and the specific conditions used in each study.

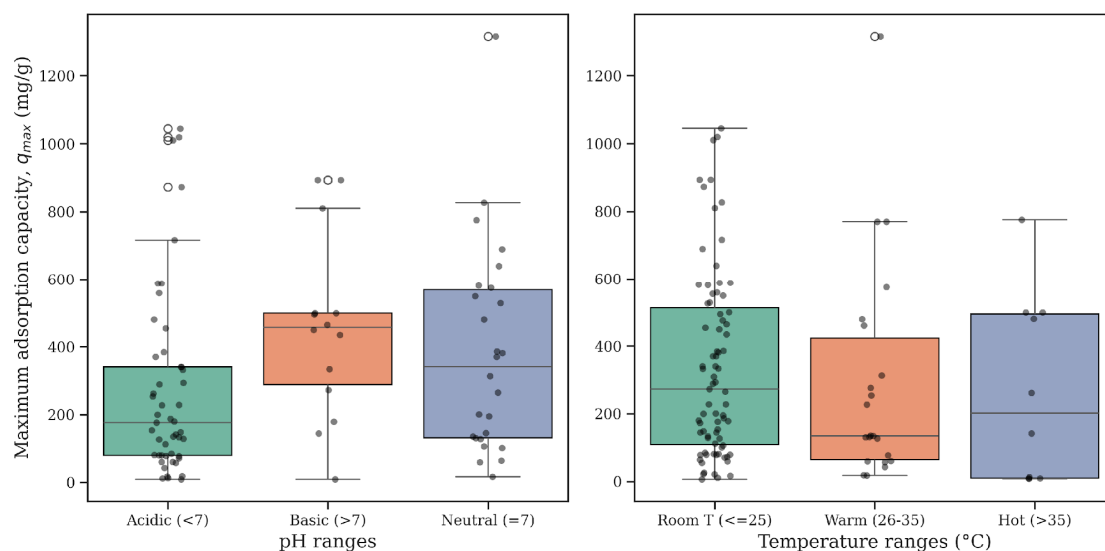


Figure 11. Boxplot distribution of maximum adsorption capacity (q_{max} , mg g^{-1}) under different pH (**left**) and temperature ranges (**right**). The figure highlights the broad distribution of adsorption capacities reported across different pH and temperature conditions. Individual points represent data reported in the selected studies. Grey, semi-transparent circles represent every individual, raw data point from the extracted dataset. White (or hollow) circles represent the statistical outliers (liers) calculated by the standard boxplot algorithm.

4. Conclusions

This study presented a PRISMA-guided bibliometric and statistical analysis of MOF-based adsorbents for organic dye removal, covering publications from 2014 to 2026. The results confirmed sustained research growth and highlighted the increasing relevance of MOFs for wastewater treatment applications. Research activity was primarily concentrated in Asia, with strong collaborative patterns across institutions.

From a materials perspective, pristine MOFs dominated the literature; however, a transition toward functionalized and composite materials was identified, driven by the need to improve adsorption efficiency, selectivity, and stability. MIL-, UiO-, and ZIF-type frameworks were the most frequently investigated due to their balance between structural stability and adsorption performance. Importantly, this work provides a benchmarking framework that integrates material classification, dye taxonomy, and adsorption performance under different operational conditions. Although functionalized MOFs frequently exhibited higher adsorption capacities within the analyzed dataset, exploratory Kruskal–Wallis analyses indicated that differences among pristine, functionalized, and composite materials were not statistically significant at the 95% confidence level. The analysis identified critical limitations in the literature, particularly the inconsistent reporting of key experimental parameters such as pH, temperature, surface area, and pore aperture, which limits comparability and hinders the identification of reliable structure–property relationships. Future studies would benefit from greater standardization in data reporting. At a minimum, key experimental parameters such as dye identity and classification, initial dye concentration, solution pH, temperature, contact time, adsorbent dosage, adsorption capacity (q_e and/or q_{max}), kinetic and isotherm model parameters, regeneration performance, and wastewater matrix composition should be consistently reported. Improved reporting practices would enhance reproducibility and facilitate more robust benchmarking analyses across MOF-based adsorption systems. Future research should focus on standardizing experimental reporting and expanding the diversity of MOF compositions and ligand chemistries, enabling more robust comparisons and supporting the rational

design of next-generation adsorbents for real wastewater applications. Beyond adsorption capacity, adsorption kinetics and regeneration performance were also identified as critical parameters for practical implementation. The majority of the analyzed studies reported adsorption behavior that was adequately described by pseudo-second-order kinetics, whereas regeneration assessments were frequently limited to a small number of cycles and often lacked standardized capacity-retention data. These limitations highlight the need for more comprehensive evaluation of MOF performance beyond $q_{\max}$ values alone. An additional challenge for the practical implementation of MOF-based adsorbents is their performance under realistic wastewater conditions. Most studies were conducted using simplified aqueous systems, whereas real wastewaters contain competing ions, dissolved organic matter, and complex chemical matrices that may reduce adsorption efficiency and alter adsorption mechanisms. Therefore, future research should place greater emphasis on evaluating MOF performance under realistic operating conditions to better assess their applicability for large-scale wastewater treatment.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/colorants5030025/s1>. Figure S1. PRISMA flow diagram illustrating the study selection process. Figure S2. Annual scientific production on MOF-based adsorption of organic dyes. Figure S3. Frequency distribution of metal nodes used in MOF-based adsorbents for dye removal. Figure S4. Distribution of regeneration cycles reported for MOF-based adsorbents used in dye removal. Table S1. Search and study selection criteria. Table S2. Database compiled using PRISMA methodology. Table S3. Descriptive statistics and Kruskal-Wallis analysis for $q_{\max}$ according to material class. Table S4. Descriptive statistics and exploratory Kruskal-Wallis analysis of $q_{\max}/SB_{\text{BET}}$ according to material class. References [50–98] are cited in supplementary materials.

Author Contributions: Conceptualization, A.M.C.-D. and N.E.D.-G.; methodology, A.M.C.-D.; software, A.M.C.-D. and J.J.A.-T.; validation, A.M.C.-D. and N.E.D.-G.; formal analysis, A.M.C.-D. and N.E.D.-G.; investigation, A.M.C.-D.; resources, N.E.D.-G.; data curation, A.M.C.-D.; writing—original draft preparation, A.M.C.-D.; writing—review and editing, N.E.D.-G.; visualization, A.M.C.-D. and J.J.A.-T.; supervision, N.E.D.-G.; project administration, N.E.D.-G.; funding acquisition, N.E.D.-G. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by SECIHTI (Secretaría de Ciencia, Humanidades, Tecnología e Innovación), grant number 592501.

Data Availability Statement: The raw data supporting the conclusions of this article will be made available by the authors on request.

Acknowledgments: The authors acknowledge the support provided by Universidad Autónoma de Nuevo León (UANL) and the Facultad de Ciencias Químicas for providing the space and facilities for the development of this research.

Conflicts of Interest: The authors declare no conflicts of interest. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript; or in the decision to publish the results.

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