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# Next-Generation Adsorbents for Wastewater Remediation: A Nanotechnology-Driven and AI-Enabled Breakthrough Towards Clean Water

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**Abstract** **Review Article**

Industrial, agricultural, and pharmaceutical water pollution still poses world health and ecosystem risks. Adsorption as a form of remediation has become popular because it requires minimum operations and is efficient in most of the pollutants. Conventional adsorbents however present the drawbacks of low selectivity, regeneration and sustainability. Through nanotechnology, this review discusses the development of the next-generation adsorbents, which have been optimised through artificial intelligence (AI) and machine learning (ML) to address such challenge. We address the more sophisticated nanomaterials- metal-organic frameworks (MOFs), carbon-based nanostructures, magnetic nanoparticles and biochar composites, and their superior surface area or porosity adjustability, and bound pollutant capacity. Means of functionalization and structural amendments are presented to enhance capacity, selectivity and durability. Predictive modeling and optimization of the adsorbent performance in practice is possible because of the integration of AI/ML instruments such as ANN, SVM, DFT, and Monte Carlo simulations. The review also includes the most important barriers such as environmental risks of nanomaterials, regeneration inefficiencies, cost performance trade-offs, and regulatory limitations. Integration of advances in materials science, data-based modeling, and sustainable engineering, this paper provides a route map toward upscale and environmentally friendly wastewater remediation. Finally, nanotechnology powered and AI enhanced adsorbents are innovations that will take the world a long way forward in the provision of clean water globally.
**Keywords:** Wastewater remediation, Advanced adsorbents, Nanotechnology-based adsorbents, Metal–organic frameworks (MOFs), Carbon-based nanomaterials (CNTs, graphene), Magnetic nanoparticles, Biochar composites, Artificial intelligence (AI), Machine learning (ML), Computational modeling (DFT, MD, Monte Carlo), Adsorption mechanisms, Water purification, Sustainable water treatment, Environmental nanotechnology, Clean water technologies.



## 1. INTRODUCTION

Wastewater management continues to be a critical challenge for both environmental sustainability and public health. Among the numerous treatment approaches, adsorption has emerged as one of the most efficient and versatile techniques, owing to its simplicity, cost-effectiveness, and ability to eliminate a wide spectrum of pollutants. Since the early 20th century, activated carbon derived from natural resources has played a pivotal role in water purification due to its capacity to remove various contaminants. Nevertheless, the growing complexity of wastewater and increasingly stringent environmental regulations demand the development of more advanced, economical, and eco-friendly alternatives [1]. The rise of nanotechnology has significantly transformed the design of adsorbent materials. By enabling manipulation at the molecular level, nanotechnology enhances pollutant capture efficiency and specificity. Advanced materials such as carbon nanotubes, graphene, metal-organic frameworks

(MOFs), and nanostructured polymers are now at the forefront, offering superior performance, selectivity, and reusability compared to conventional adsorbents. These nanoscale innovations provide the potential for targeted removal of pollutants such as heavy metals, organic compounds, pharmaceuticals, and endocrine-disrupting chemicals, setting a new benchmark in water purification strategies [2].

Equally transformative is the integration of artificial intelligence (AI) and machine learning (ML) into adsorption research. These technologies address long-standing challenges by optimizing regeneration efficiency and predicting adsorption behavior under diverse environmental conditions. Through AI- and ML-driven modeling, scientists can design intelligent adsorbents that adapt dynamically to their surroundings, thereby improving both efficiency and sustainability. This development opens new avenues for solving complex wastewater treatment issues. Alongside these advances, sophisticated analytical techniques such as scanning electron microscopy (SEM) and high-performance liquid chromatography (HPLC) have provided deeper insights into the physicochemical interactions between adsorbents and pollutants. Such progress enriches our understanding of adsorption mechanisms and supports the optimization of this essential technology [3–5].

The global shift toward low-carbon strategies, emphasizing energy conservation and resource recycling, introduces additional challenges for conventional wastewater treatment systems [6]. Although modern adsorption technologies offer significant promise, their large-scale application is hindered by issues such as scalability, cost management, and the safe production and disposal of adsorbent materials [7]. Moreover, the potential ecological and health risks associated with nanomaterials warrant thorough evaluation. Addressing these obstacles calls for a multidisciplinary effort involving material science, environmental engineering, toxicology, and regulatory frameworks [8].

This review highlights recent breakthroughs in material science and nanotechnology, supported by AI and ML, that are advancing adsorption-based wastewater treatment. It further examines the economic and environmental implications of these innovations while outlining future directions for the field. By demystifying complex technologies and their applications, this review aims to demonstrate how these advancements contribute to sustainable and effective wastewater purification, underscoring their broader importance for environmental health and sustainability.

## 2. Historical Analysis of Adsorption Techniques

Adsorption refers to the process in which molecules of an adsorbate adhere to the surface of an adsorbent through intermolecular forces. This phenomenon has been extensively applied in wastewater treatment to remove a wide range of contaminants, including organic pollutants, heavy metals, dyes, nutrients, and pathogens [9]. The use of adsorption in water purification dates back to the late 19th century, with the first patent for an activated carbon filter granted to R. V. Ostrejko in 1900 [1]. Since then, activated carbon has remained a widely utilized adsorbent due to its high surface area, porosity, and strong affinity for organic molecules.

Despite its effectiveness, activated carbon presents certain limitations, such as high production costs, limited selectivity, and challenges in regeneration [10]. To address these shortcomings, researchers have investigated a variety of alternative adsorbents, including natural materials (e.g., clay, zeolite, biomass), synthetic materials (e.g., silica gel, metal oxides, polymers), and hybrid systems (e.g., metal-organic frameworks, carbon nanotubes, graphene oxide). These materials offer distinct advantages over conventional activated carbon, such as enhanced adsorption capacity, greater selectivity, improved stability, reusability, and cost-effectiveness.

The continuous advancement of adsorption technologies has been largely driven by the growing global demand for clean water and increasingly strict environmental regulations, which emphasize the need for efficient and sustainable wastewater treatment strategies [11,12].

## 3. Notable Progress in the Last Decade

Over the past decade, significant progress has been made in enhancing the adsorption efficiency and specificity of newly developed adsorbents, along with an improved understanding of adsorption mechanisms and kinetics. A key breakthrough in this field has been the application of nanotechnology, which enables the synthesis of nanoscale materials with distinctive properties, such as exceptionally high surface area, tunable pore size and geometry, and the presence of functional groups. These nanomaterials can be employed either as independent adsorbents or as core components in composite systems. Widely investigated nanomaterials for adsorption applications include carbon nanotubes, graphene, metal oxides, metal-organic frameworks (MOFs), zeolites, and magnetic nanoparticles [13]. Their remarkable adsorption capacities stem from their large surface areas and the potential for specific interactions with pollutants. For example, carbon nanotubes can effectively remove dyes and heavy metals through π–π stacking and electrostatic interactions, while MOFs exhibit selective adsorption of organic molecules and nutrients via coordination bonding and molecular sieving [14,15].

Another important advancement lies in the modification of both natural and synthetic materials to enhance their adsorption performance. Such modifications may involve physical treatments (e.g., thermal activation, acid or base washing, irradiation), chemical methods (e.g., impregnation, grafting, coating), or biological approaches (e.g., biosorption, biochar production). These treatments can alter key surface characteristics of adsorbents—including surface area, porosity, charge, hydrophobicity, and functional groups—thereby improving their overall efficiency [16].

The development of novel adsorbents and modification techniques has been supported by the progress of analytical methods and theoretical modeling, which provide deeper insights into adsorption processes. Analytical techniques reveal crucial physicochemical properties of both adsorbents and pollutants, such as surface morphology, elemental composition, pore size distribution, charge, functional groups, molecular structure, and solubility. Commonly applied methods include SEM, TEM, XRD, XPS, FTIR, NMR, TGA, BET surface analysis, zeta potential measurements, UV–Vis spectroscopy, and HPLC. These tools help identify the dominant factors influencing adsorption, such as surface area, pore size, functional groups, polarity, molecular size, and pH [5]. *Figure 1* presents the main classes of adsorbents, summarizing their key properties and the characterization methods employed.

In parallel, theoretical models have advanced to better describe and predict adsorption behavior under various conditions. These models are generally categorized as equilibrium or kinetic. Equilibrium models, such as the Langmuir, Freundlich, Temkin, and Dubinin–Radushkevich isotherms, describe the relationship between the amount of pollutant adsorbed and its equilibrium concentration in solution. They provide insights into maximum adsorption capacity, adsorption strength, associated heat changes, and the nature of the process. Kinetic models, including the pseudo-first-order, pseudo-second-order, intraparticle diffusion, and Elovich models, explain the rate at which pollutants are adsorbed, taking into account factors such as mass transfer, diffusion, and reaction. These models yield critical parameters such as rate constants, equilibrium uptake, diffusion coefficients, and activation energies [17].

Figure 1 illustrates the taxonomy of modern adsorbents—spanning nanomaterials (e.g., carbon nanotubes, graphene, MOFs, magnetic nanoparticles), natural/synthetic bases, and hybrid formulations—along with common modification methods (physical, chemical, biological) and key characterization tools (SEM, TEM, XRD, FTIR, BET, etc.). This diagram emphasizes the interconnected evolution of materials, treatment strategies, and analytical techniques driving adsorption innovation.

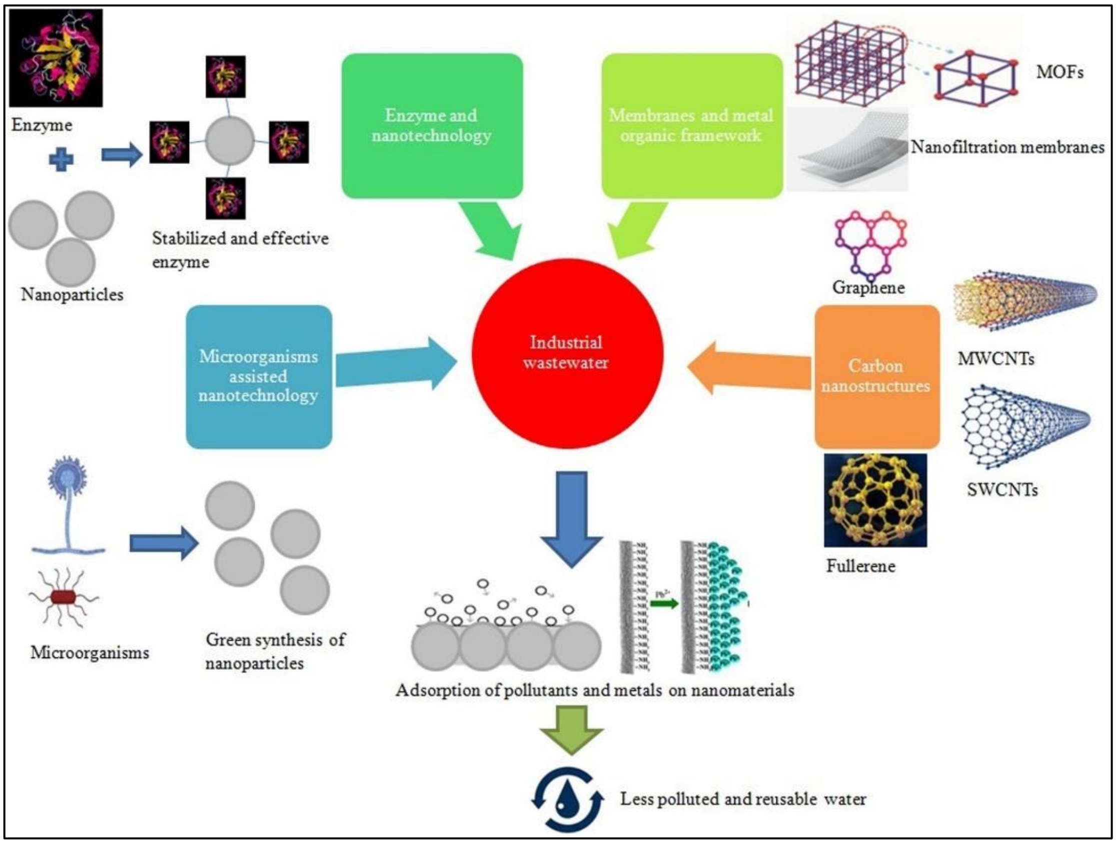



**Figure1: Classification of Advanced Adsorbents, Their Surface Modifications, and Characterization Techniques"**

Figure 1 provides a schematic classification of advanced adsorbents used in wastewater treatment. It highlights major categories, including natural adsorbents (e.g., clay, zeolite, biomass), synthetic materials (e.g., silica gel, polymers, metal oxides), and emerging nanomaterials such as carbon nanotubes, graphene, MOFs, and magnetic nanoparticles. The figure also outlines surface modification strategies—physical (thermal activation, irradiation), chemical (impregnation, grafting, coating), and biological (biosorption, biochar production)—which enhance surface properties like porosity, charge, hydrophobicity, and functional groups.

Additionally, the figure integrates the principal analytical and characterization techniques—such as SEM, TEM, XRD, FTIR, BET, NMR, and HPLC—used to evaluate adsorbent structure and performance. Together, these elements emphasize the interplay of material innovation, modification strategies, and analytical insights that have shaped adsorption science in the past decade, paving the way for efficient and sustainable wastewater purification.

## 4. Detailed Analysis of Current Limitations

Despite significant advancements in adsorption-based wastewater treatment, several challenges remain that hinder large-scale application. These limitations can be broadly grouped into six categories: adsorption capacity, selectivity and non-specific binding, material degradation and stability, recovery and reusability of adsorbents, economic feasibility, and regulatory as well as environmental concerns. Each of these is discussed in detail below.

### 4.1. Adsorption Capacity

Adsorption capacity plays a critical role in determining the efficiency and effectiveness of adsorption processes in wastewater treatment. It refers to the amount of adsorbate that a specific mass of adsorbent can capture under defined conditions. This capacity is affected by multiple factors (Table 1), including adsorbent characteristics (surface area, porosity, functional groups), adsorbate properties (molecular size, polarity, concentration), and operational conditions (temperature, pH, and contact time) [2,18].

A major limitation is that the adsorption capacity of most existing adsorbents remains relatively low when compared with the high concentration and diversity of contaminants in wastewater. Consequently, large quantities of adsorbents are required to achieve effective removal, increasing both cost and operational complexity. In addition, adsorption capacity typically decreases with higher initial adsorbate concentrations, as available binding sites on the adsorbent surface become saturated [19]. Hence, there is an urgent need to design and develop novel adsorbents with improved adsorption capacity and stronger affinity toward diverse wastewater contaminants.

**Table 1: Key Factors Influencing Adsorption Capacity**

| Category | Factors | Limitations |
|---|---|---|
| Adsorbent characteristics | Surface area, porosity, functional groups | Many adsorbents still show low capacity |
| Adsorbate properties | Molecular size, polarity, concentration | High concentrations lead to site saturation |
| Operational conditions | Temperature, pH, contact time | Performance drops under non-optimal conditions |

### 4.2 Selectivity and Non-Specific Binding

The selectivity of an adsorbent is another key factor in determining its suitability for wastewater treatment. Selectivity is defined as the ability of an adsorbent to preferentially capture and retain a target pollutant from a mixture of substances. It is influenced by factors such as surface chemistry, pore size distribution, and functional groups of the adsorbent, as well as the molecular size, polarity, charge, and geometry of the adsorbates. Operational parameters, including pH, temperature, and ionic strength, also play a role [20].

Achieving high selectivity, however, remains difficult given the complexity of wastewater compositions. For example, activated carbon—one of the most widely used adsorbents—can remove a broad range of organic pollutants through interactions such as hydrophobic forces, $\pi$–$\pi$ stacking, hydrogen bonding, and electrostatic attraction. Yet, these same interactions also attract water molecules and other polar compounds, thereby reducing selectivity for target pollutants [21]. Another challenge is competitive adsorption, where multiple adsorbates compete for limited binding sites. At higher concentrations of pollutants, competition intensifies, leading to diminished selectivity. Addressing this issue requires careful optimization of operating conditions and the judicious selection of adsorbent materials to strike a balance between selectivity and efficiency [22]. *Figure 2* highlights the major factors that govern adsorbent selectivity in wastewater remediation.

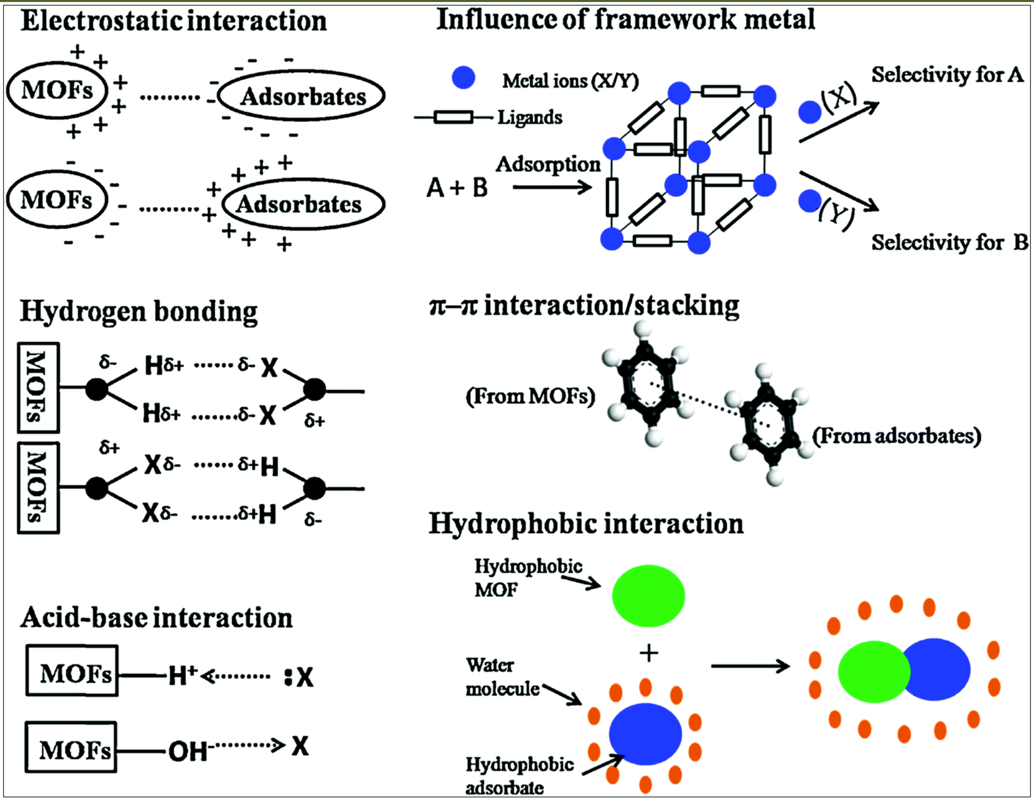



**Figure 2. Critical Factors Influencing Adsorbent Selectivity and Non-Specific Binding in Wastewater Treatment**

Figure 2 maps the key drivers of selective adsorption—surface chemistry, pore architecture, and functional groups—together with operational parameters (pH, temperature, ionic strength). It highlights how adsorbent–adsorbate interactions (electrostatic attraction, hydrogen bonding, acid–base pairing, π–π stacking, hydrophobic effects) govern specificity. The graphic also reflects non-specific binding and competition for limited sites under complex matrices. Overall, it captures why optimizing both material design and conditions is essential for high selectivity.

### 4.2. Material Degradation and Stability

Material degradation and stability describe an adsorbent's ability to retain its structural integrity, function, and performance under diverse operational and environmental conditions [23]. Stability depends on several parameters, including adsorbent properties (chemical composition, crystallinity, morphology), adsorbate characteristics (acidity, redox potential, biodegradability), and operating conditions (temperature, pH, and contact time) [24].

A persistent limitation is that many adsorbents exhibit inadequate stability when exposed to the harsh and complex environments typical of wastewater treatment. Extended contact times and repeated use often exacerbate degradation, leading to physical or chemical deterioration of the adsorbent's surface and structure [25]. This reduces long-term efficiency and underscores the necessity of designing more durable and stable adsorbent materials.

### 4.3. Recovery and Reusability of Adsorbents

Recovery and reusability refer to an adsorbent's ability to be separated from treated water and reused in subsequent adsorption cycles following regeneration. These properties depend on multiple factors, including the intrinsic characteristics of the adsorbent (density, magnetic properties, shape, and size), the nature of the adsorbate (solubility, biodegradability, toxicity), and operational conditions such as pH, temperature, and contact time [26].

A persistent challenge in adsorption-based treatment is that the recovery and reusability of most adsorbents remain limited compared with the scale and frequency of wastewater treatment needs. Reusability often declines due to fouling of the adsorbent surface or pore blockage by organic matter or inorganic precipitates [23]. Magnetic adsorbents address some of these limitations by enabling rapid and efficient separation using an external magnetic field, which reduces energy requirements and minimizes adsorbent loss. They have also demonstrated strong adsorption performance for diverse micropollutants, including dyes, heavy metals, pharmaceuticals, pesticides, and organic compounds [27].

Nonetheless, practical deployment of magnetic adsorbents is constrained by several issues. These include reduced stability under variable environmental conditions (pH, salinity, temperature, redox potential), which may affect both their magnetic properties and adsorption capacity [28]; the influence of regeneration techniques on recovery efficiency [29]; and concerns regarding ecotoxicological risks to aquatic ecosystems and human health [30,31]. *Figure 3* summarizes the principal challenges in magnetic adsorption technology, focusing on stability, synthesis, regeneration, and ecological safety.

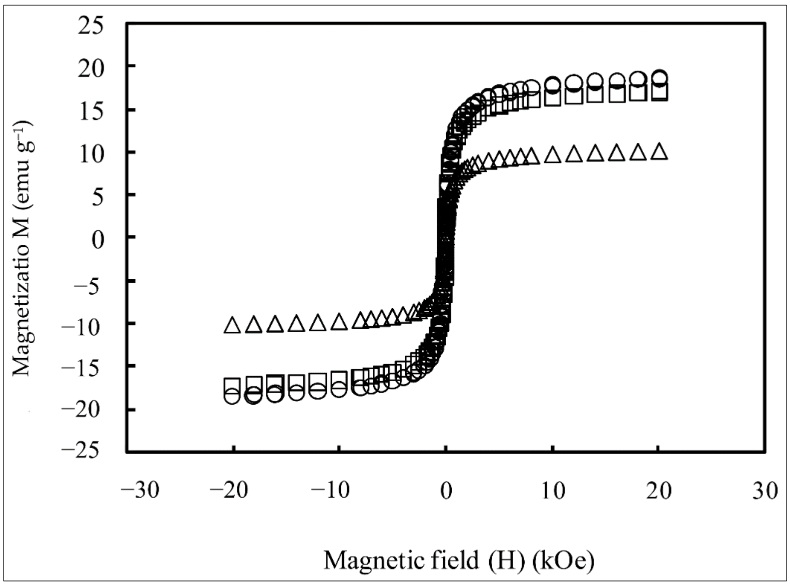



**Figure 3: Key Challenges in the Recovery and Reusability of Magnetic Adsorbents for Wastewater Treatment**

Figure 3 highlights the critical factors influencing the recovery and reusability of magnetic adsorbents. While magnetic properties allow efficient separation and reuse through external fields, several challenges persist. These include material instability under varying pH, salinity, temperature, and redox conditions; reduced efficiency due to fouling and regeneration limitations; and potential ecotoxicological risks to aquatic systems and human health. The figure underscores the need for stable, sustainable, and safe designs to maximize the long-term applicability of magnetic adsorption technology.

### 4.4. Economic Viability

The long-term adoption and sustainability of adsorption processes in wastewater treatment depend heavily on their economic feasibility. Although adsorption is considered simple, efficient, and highly selective compared with conventional treatment methods, its economic limitations remain a critical barrier. Costs are strongly influenced by adsorbent source, preparation method, and surface modification. Activated carbon, for instance, is widely used but remains relatively expensive due to its energy-intensive production process. To address this issue, alternative low-cost adsorbents derived from agricultural and industrial by-products, such as chitosan, zeolites, and activated clays, have been proposed as promising substitutes [2,32].

Wastewater properties also significantly impact cost-effectiveness. Streams with high pollutant concentrations or diverse contaminant profiles often require larger amounts of adsorbent, thereby increasing operational expenses. Additionally, the presence of toxic compounds can necessitate more frequent regeneration or careful disposal of spent adsorbents, further adding to treatment costs [2].

### 4.5. Regulatory and Environmental Challenges

Another key limitation in adsorption-based wastewater treatment relates to regulatory and environmental challenges surrounding the use, management, and disposal of adsorbents. On the regulatory side, there is a lack of standardized guidelines regarding adsorbent quality, performance, and safety, as well as monitoring protocols for their application [33]. Variations in national and regional regulatory frameworks create uncertainties for manufacturers, suppliers, and end-users. Furthermore, lengthy and costly approval processes may hinder innovation and the commercialization of novel adsorbent materials. To overcome these barriers, there is a strong need for harmonized and streamlined regulatory frameworks at both national and international levels, along with awareness-building initiatives to educate stakeholders on the risks and benefits of adsorbent technologies [34,35].

From an environmental perspective, concerns focus on the potential impacts of adsorbents across their life cycle, including production, application, recycling, and final disposal. Such impacts may pose risks to both human health and environmental systems if not properly managed, underscoring the importance of safe design, regulation, and eco-friendly disposal pathways.

**Table 2: Regulatory and Environmental Challenges of Adsorption-Based Wastewater Treatment**

| Category | Key Issues | Implications |
|---|---|---|
| Regulatory | Lack of standardized guidelines for adsorbent quality, performance, and safety. | Creates uncertainty for manufacturers, suppliers, and users. |
| | Variations across national and regional frameworks. | Difficulties in global commercialization and technology transfer. |
| | Lengthy, costly, and complex approval processes. | Slows down innovation and adoption of novel adsorbents. |
| | Limited awareness among stakeholders. | Hinders effective implementation and acceptance of new technologies. |
| Environmental | Risks across the life cycle (production, use, recycling, and disposal). | Potential harm to human health and ecosystems. |
| | Fouling and hazardous by-products during application. | Increases treatment and disposal challenges. |
| | Poor disposal or lack of recycling pathways. | Long-term environmental burden and contamination risk. |
| | Need for eco-friendly and sustainable design approaches. | Encourages development of greener, safer adsorbents. |

## 5. Advances to Overcome Current Limitations

Although substantial progress has been made in developing innovative adsorbents for water purification, several limitations remain that must be addressed to improve their performance and broaden their applicability. Section 4 identified these challenges, and the following subsections discuss recent breakthroughs aimed at overcoming them, along with potential directions for future advancement.

### 5.1. Adsorption Capacity

Recent studies have placed significant emphasis on designing novel adsorbents with enhanced adsorption capacity for contaminant removal. Nanostructured materials such as carbon nanotubes (CNTs), MOFs, and graphene, with their exceptionally high surface areas, offer abundant binding sites for adsorbate molecules. Tailored pore structures, including mesoporous and hierarchical frameworks, further promote size-exclusion effects, enabling selective capture of contaminants. Beyond surface area, these materials also provide specific chemical interactions and nanoconfinement effects, which substantially strengthen adsorption performance. Such properties open new possibilities for addressing pollutants that were previously difficult to remove [21,39].

Computational tools have also emerged as powerful aids in screening large databases of candidate materials, particularly MOFs, to identify the most efficient adsorbents. Owing to their tunable porosity and adjustable chemical properties, MOFs demonstrate high potential in water treatment applications [40].

Ensuring consistent adsorption under diverse physicochemical conditions remains challenging. Nonetheless, several materials show resilience across wide operational ranges. Activated carbon, with its extensive surface area and varied functional groups, is highly effective in adsorbing organic pollutants over different pH levels [41]. Modified clays and zeolites offer tunable pore structures and surface charges that enable targeted adsorption under fluctuating pH conditions [42,43]. MOFs exhibit exceptional versatility due to their customizable frameworks and metal centers, which allow selective adsorption across a range of pH and temperature conditions [44]. Likewise, biopolymer-based adsorbents, derived from chitosan and cellulose, display strong stability and naturally bind heavy metals through inherent functional groups [45,46].

Functionalization techniques represent another key advancement, enabling the incorporation of targeted functional groups that enhance interactions with specific contaminants, whether organic or inorganic. This targeted approach increases both selectivity and overall adsorption efficiency [47]. Collectively, these innovations are improving not only adsorption performance but also the cost-effectiveness and sustainability of wastewater treatment.

### 5.2. Selectivity and Non-Specific Binding

Efforts to address challenges of selectivity and non-specific binding have resulted in significant advances in adsorbent design, particularly within chemical, environmental, and biological engineering. Molecularly Imprinted Polymers (MIPs) are among the most promising developments. Fabricated using template molecules, MIPs generate cavities that mimic the size and functional groups of the target contaminant, thereby enabling high selectivity and minimizing non-specific interactions [48].

Inorganic molecular imprints, such as those on titanium dioxide and silica-titania composites, further enhance resilience, offering superior thermal and chemical stability compared to organic systems—an advantage in extreme environments [49,50]. Single-crystal surface imprinting represents another innovation, employing flat and rigid crystal substrates (such as metal oxides and MOFs) to create high-quality recognition sites with reduced non-specific adsorption [51].

Other strategies focus on exploiting specific interaction mechanisms. Hydrophobic adsorbents selectively capture non-polar molecules from aqueous environments, making them valuable for oil spill remediation [52]. Electrostatic tailoring allows adsorbents to bind charged pollutants, aiding in the removal of ionic dyes and similar contaminants [53]. Acid–base surface modifications create active sites that interact with electron-donating or -accepting pollutants [54]. Moreover, adsorbents with tunable redox-active surfaces can be designed to promote selective redox interactions with target pollutants, further enhancing specificity [55].

Together, these advancements represent major progress in overcoming the long-standing limitations of selectivity and non-specific binding, offering new pathways for high-performance water remediation.

### 5.3. Material Degradation and Stability

Although adsorbents play a critical role in pollutant removal, their performance is often limited by instability and degradation under operational conditions. Recent advances focus on strengthening structural resilience against physicochemical stressors. For activated carbon, surface modifications have been developed to enhance oxidation resistance and improve adsorption efficiency. MOFs have benefited from the introduction of hydrophobic functional groups and specialized linkers, addressing structural collapse issues.

For zeolites, strategies such as hydrothermal stabilization and silylation are used to prevent dealumination, while polymer resins achieve greater durability through crosslinking and imprinting techniques. Biosorbents now incorporate chemical modifications and immobilization approaches to improve biodegradation resistance. Silica gels have been stabilized with organosilane grafting, and alumina's thermal stability has been strengthened using sol-gel synthesis and doping. Similarly, CNTs and graphene oxide retain their performance through functionalization and reduction methods.

These innovations are summarized in *Table 2*, which outlines the main challenges and recent strategies aimed at enhancing stability across different adsorbent classes. Such multidisciplinary approaches highlight the importance of integrating materials science, chemistry, and environmental engineering to improve durability in water treatment applications.

### 5.4. Recovery and Reusability of Adsorbents

Recovery and reusability remain significant barriers to large-scale adoption of adsorption technologies. Conventional recovery methods such as centrifugation, filtration, and sedimentation often prove inefficient, energy-intensive, or laborious due to additional processing steps. To address these limitations, innovative strategies are being developed to improve separation and extend adsorbent lifespan.

One promising approach is the stabilization of magnetic properties over multiple reuse cycles. Covalent immobilization of biopolymers onto particle surfaces enhances bonding strength, minimizes leaching, and maintains high adsorption efficiency during repeated regeneration [65]. Similarly, embedding magnetite nanoparticles within biopolymer matrices has led to biosorbents with excellent pollutant removal performance and easy recovery using magnets. These materials have proven effective against a variety of contaminants, including heavy metals and dyes [66].

The integration of natural polymers such as chitosan, carrageenan, and cellulose into magnetic nanocomposites is another promising strategy. These biopolymer-based composites are not only biodegradable and environmentally safe but also mechanically reinforced through crosslinking with magnetic nanoparticles, increasing both stability and durability [67].

Innovative frameworks such as covalent organic framework (COF)-chitosan aerogels have been developed using hierarchical architectures and dual crosslinking strategies. These floating aerogels, with high porosity and low density, are easily recoverable and have achieved impressive pollutant removal capacities (e.g., 102.5 mg/g of sulfamerazine) [68,69]. Additionally, combining adsorbents with membranes represents another promising approach. Immobilizing adsorbents on membrane surfaces enables direct water contact while facilitating easy backwashing for regeneration. Hollow fiber membranes filled with adsorbents create compact systems that improve separation efficiency and simplify reusability [70,71].

### 5.5. Economic and Ethical Challenges

Addressing economic and ethical concerns has become central to advancing adsorption-based water treatment. Economic feasibility depends heavily on reducing synthesis and operational costs. Advances in green chemistry have promoted the production of low-cost, high-performance adsorbents through sustainable methods that minimize energy consumption and reduce reliance on hazardous or expensive precursors. Techniques such as sol-gel processing, hydrothermal synthesis, and bio-fabrication are now optimized for efficiency, ensuring high adsorption performance while lowering costs [72].

From an ethical perspective, the environmental footprint of adsorbents has prompted the integration of circular economy principles into their design. This includes the use of biodegradable materials, improved regeneration processes, and strategies to extend adsorbent lifespans through surface modification and composite engineering [73].

Technological innovations have also produced hybrid systems that integrate adsorption with advanced treatment processes, such as membrane filtration and photocatalysis. These systems combine synergistic mechanisms to enhance efficiency, reduce secondary pollutants, and improve selectivity [74].

Finally, advanced evaluation tools such as life cycle assessment (LCA) and cost–benefit analysis (CBA) have been increasingly applied to assess the sustainability and economic feasibility of adsorbent technologies. By quantifying environmental impacts and treatment costs, these tools support evidence-based decision-making. Surrogate-based optimization methods are also being used to balance cost-effectiveness with treatment performance, accelerating the transition from laboratory-scale research to market-ready solutions [75].

## 6. Case Studies of Novel Approaches

Recent years have witnessed remarkable progress in adsorption technologies for water remediation, with several novel strategies demonstrating enhanced efficiency and sustainability. These include biochar-based adsorbents, nanomaterials, metal–organic frameworks (MOFs), hybrid composites, and membrane-assisted adsorption systems. Additionally, modern computational tools such as artificial intelligence (AI) and machine learning (ML) are increasingly applied to optimize adsorption performance. The following subsections present key innovations and highlight their contributions to water purification.

### 6.1. Biochar-Based Adsorbents

Biochar has emerged as a versatile adsorbent owing to its abundance, low cost, and modifiable properties. Recent approaches have focused on enhancing its physical and chemical characteristics through steam activation, thermal air treatment, acid modification, and the fabrication of biochar nanocomposites. Techniques such as ball milling and surface functionalization have further improved its adsorption efficiency. Magnetic biochar represents another major advancement, enabling simple recovery and reuse while significantly boosting pollutant removal. *Table 3* summarizes recent innovations and outcomes in the field of biochar-based adsorbents, emphasizing their versatility in water remediation.

**Table 3: Biochar-Based Adsorbents for Water Remediation**

| Method | Modification/Approach | Performance Outcome |
|---|---|---|
| Steam/thermal activation | Enhanced porosity and surface reactivity | Increased adsorption efficiency |
| Acid modification | Introduction of functional groups | Improved affinity for heavy metals/dyes |
| Biochar nanocomposites | Combination with nanoparticles | Higher capacity and stability |
| Magnetic biochar | Magnetic recovery and reuse | Efficient separation and pollutant removal |

### 6.2. Nanomaterials in Adsorption

Nanotechnology has revolutionized adsorption science by enabling the design of nano-adsorbents with high capacity, fast kinetics, and strong pollutant selectivity. Advances include green synthesis routes, magnetic nanoparticle composites, and bio-inspired designs, each contributing to improved sustainability and adsorption performance. These engineered nanomaterials exhibit remarkable efficiency across a wide spectrum of contaminants, from heavy metals to pharmaceuticals. *Table 4* presents an overview of notable nanomaterial-based adsorbents, their unique features, and pollutant removal efficiencies.

**Table 4: Nanomaterial-Based Adsorbents in Water Treatment**

| Nanomaterial Type | Approach | Key Benefits |
|---|---|---|
| CNTs/Graphene | Surface functionalization, green synthesis | High adsorption capacity, rapid kinetics |
| Magnetic nanoparticle composites | Magnetic recovery, hybridization | Easy reuse, improved performance |
| Bio-inspired nanomaterials | Natural-mimicking fabrication | Enhanced selectivity and sustainability |

### 6.3. Metal–Organic Framework (MOF)-Based Adsorbents

MOFs have attracted extensive research attention due to their tunable porosity, high surface area, and structural versatility. Recent case studies report innovative synthesis and functionalization strategies, including aerogel composites, bio-nanocomposite beads, bimetallic MOFs, and amorphous MOFs prepared using deep eutectic solvents. These approaches have delivered significant improvements in adsorption capacity, selectivity, and environmental stability. *Table 5* summarizes recent MOF-based developments, highlighting synthesis routes, performance outcomes, and their implications for wastewater treatment.

**Table 5: MOF-Based Adsorbents for Water Remediation**

| MOF Type/Approach | Innovation | Outcome |
|---|---|---|
| Aerogel composites | Lightweight porous networks | High adsorption capacity, easy handling |
| Bio-nanocomposite beads | Integration with biopolymers | Improved selectivity and recyclability |
| Bimetallic MOFs | Dual-metal centers | Enhanced stability and performance |
| Amorphous MOFs (DES route) | Deep eutectic solvent synthesis | Superior adsorption under variable conditions |

### 6.4. Membrane-Based Adsorption Techniques

The integration of adsorption with membrane separation has given rise to hybrid systems that enhance both efficiency and selectivity in water purification. Membrane-based adsorption systems have proven effective for removing heavy metals, organic compounds, and emerging contaminants. Innovations include functionalized membranes, novel adsorptive coatings, and hybrid membrane–adsorbent assemblies, all of which contribute to improved adsorption capacities, stability, and reusability. *Table 6* outlines key membrane-based adsorption strategies, their fabrication methods, and pollutant removal efficiencies.

**Table 6: Membrane-Based Adsorption Techniques**

| Approach | Innovation | Performance Benefit |
|---|---|---|
| Functionalized membranes | Surface coating with adsorbents | Enhanced selectivity and reusability |
| Hybrid membrane–adsorbent systems | Hollow fiber and layered composites | Improved separation and regeneration |
| Adsorptive coatings | Integration of nanomaterials onto membranes | Increased adsorption capacity, durability |

### 6.5. Machine Learning and AI in Adsorption Optimization

The integration of Machine Learning (ML), Artificial Intelligence (AI), and computational approaches such as molecular simulations into water treatment—particularly adsorption technologies—represents a transformative advancement in environmental engineering. These methodologies have significantly improved the precision and efficiency of identifying and optimizing adsorbents for pollutant removal [4].

The workflow of AI/ML projects typically involves problem formulation, dataset construction, model training, evaluation, and deployment. It begins with analyzing available data to guide model and algorithm selection. Dataset construction entails data collection, inspection, processing, and visualization to ensure model reliability. Model training relies on iterative optimization to minimize the loss function, thereby improving predictive accuracy. Evaluation metrics, including Mean Absolute Error (MAE) and Root Mean Square Error (RMSE), validate performance across training and test datasets, distinguishing between regression and classification models. Issues such as overfitting and underfitting are mitigated through techniques like parameter regularization and cross-validation, which enhance generalizability [119]. *Figure 4* illustrates a typical workflow for applying ML models in adsorption optimization.

Molecular simulations also play a crucial role in advancing adsorption studies. Density Functional Theory (DFT) has been particularly valuable in predicting adsorbent capacity and elucidating adsorption mechanisms, thereby reducing the need for extensive experimental testing [120]. Complementary approaches such as Molecular Dynamics (MD) and Monte Carlo simulations extend these capabilities. MD simulations, using algorithms like Verlet and force fields such as CHARMM and AMBER, allow detailed examination of contaminant–adsorbent interactions and prediction of real-time adsorption processes. For example, MD has been applied to evaluate polyether block amide membranes, revealing the influence of cavity size on adsorption capacity. Monte Carlo simulations provide a broader statistical perspective, useful for optimizing treatment system design, though they are less effective in capturing dynamic molecular interactions [121–123].

Another valuable computational tool, Computational Fluid Dynamics (CFD), provides insights into flow dynamics and hydrodynamic behavior within treatment systems. Although CFD is highly useful for design optimization at the macroscopic scale, it is less effective in capturing atomic-level processes [121].

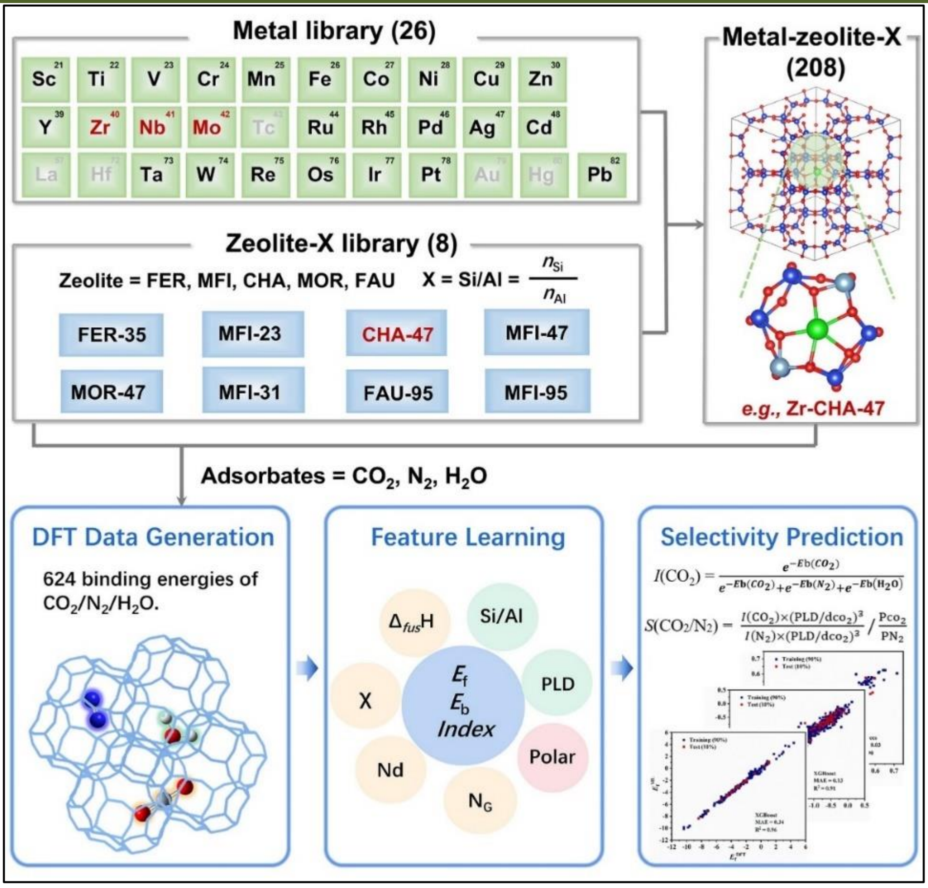



**Figure 4: Workflow and Computational Tools for Machine Learning and AI in Adsorption Optimization**

Figure 4 shows how AI/ML integrates with computational modeling to optimize adsorption. The workflow runs from dataset curation through model training/validation to prediction and deployment for performance tuning. Physics-based simulations—DFT, MD, and Monte Carlo—supply mechanistic insights and training labels; CFD informs unit design and flow behavior. Together, these tools boost predictive accuracy, cut experimental burden, and accelerate high-efficiency adsorbent discovery.

Machine learning enhances these approaches by analyzing large datasets of adsorbent characteristics and wastewater compositions to accurately predict adsorption capacities. This predictive power significantly reduces the experimental burden while improving efficiency. AI techniques such as k-Nearest Neighbor (k-NN), Decision Trees (DT), Random Forests (RF), Artificial Neural Networks (ANNs), and Support Vector Machines (SVMs) have all been widely applied in adsorption research. These models excel in regression, classification, and pattern recognition tasks. ANNs are particularly well suited for modeling complex nonlinear systems, while SVMs demonstrate strong performance in high-dimensional data analysis. Collectively, these AI and ML methods offer powerful tools for advancing adsorption optimization and wastewater treatment.

## 7. Comparative Evaluation of Adsorption Techniques

Adsorption techniques have long been explored and applied for diverse environmental applications, and their evolution reflects major progress in both materials' science and process engineering. Early approaches relied on conventional materials such as activated carbon and zeolites, which established the foundation for adsorption-based water remediation. Over time, significant advancements have introduced modern methods employing advanced materials, including carbon nanotubes and graphene-based structures [124]. Comparative evaluation of these techniques reveals a complex balance of factors—such as efficacy, efficiency, cost, and environmental impact—that together determine their suitability for specific applications. The following subsections provide a closer examination of these aspects, emphasizing recent innovations and their implications.

### 7.1. Traditional vs. Modern Adsorption Methods

In water remediation, adsorption methods have undergone substantial transformation, progressing from traditional to modern approaches as a result of advancements in environmental engineering and material science. Traditional techniques have typically used natural adsorbents, including activated carbon, clay minerals, and biochar. While effective under certain conditions, these materials are often limited by their relatively low adsorption capacity, reduced selectivity, and limited regeneration potential [47,125].

Modern adsorption methods, by contrast, integrate nanotechnology and sophisticated material synthesis. Examples include the application of carbon nanomaterials, dendritic polymers, metal oxides, and nanostructured adsorbents. These materials provide improved adsorption capacity, greater pollutant specificity, and enhanced regeneration efficiency. For instance, graphene oxide–zinc oxide nanocomposites have demonstrated strong performance in removing heavy metals from wastewater, while polysaccharide-based adsorbents offer cost-effective solutions for capturing toxic pollutants [39].

Although the principle of adsorption remains the same—based on the interaction between adsorbate and adsorbent surfaces—modern materials are often engineered with tailored functional groups and structural features that increase their affinity toward specific contaminants. This specificity is particularly critical when addressing complex wastewater streams containing diverse pollutants.

Production techniques also distinguish traditional from modern methods. Conventional adsorbents such as activated carbon are typically manufactured via physical or chemical activation, whereas modern nanostructured adsorbents often require advanced fabrication processes to achieve precise chemical and structural properties. As a result, modern adsorbents exhibit significantly higher adsorption capacities than traditional materials, primarily due to their large surface areas and engineered interaction sites [9,21].

### 7.2. Efficacy and Efficiency Evaluation

Evaluating the efficacy and efficiency of different adsorbents in water remediation is essential, particularly in light of escalating pollution levels and the demand for sustainable treatment solutions. Adsorbent-based methods are widely valued because of their strong pollutant removal capacity, straightforward synthesis, and potential economic benefits. However, their performance can vary considerably depending on the adsorbent type and the nature of the pollutants targeted for removal [129].

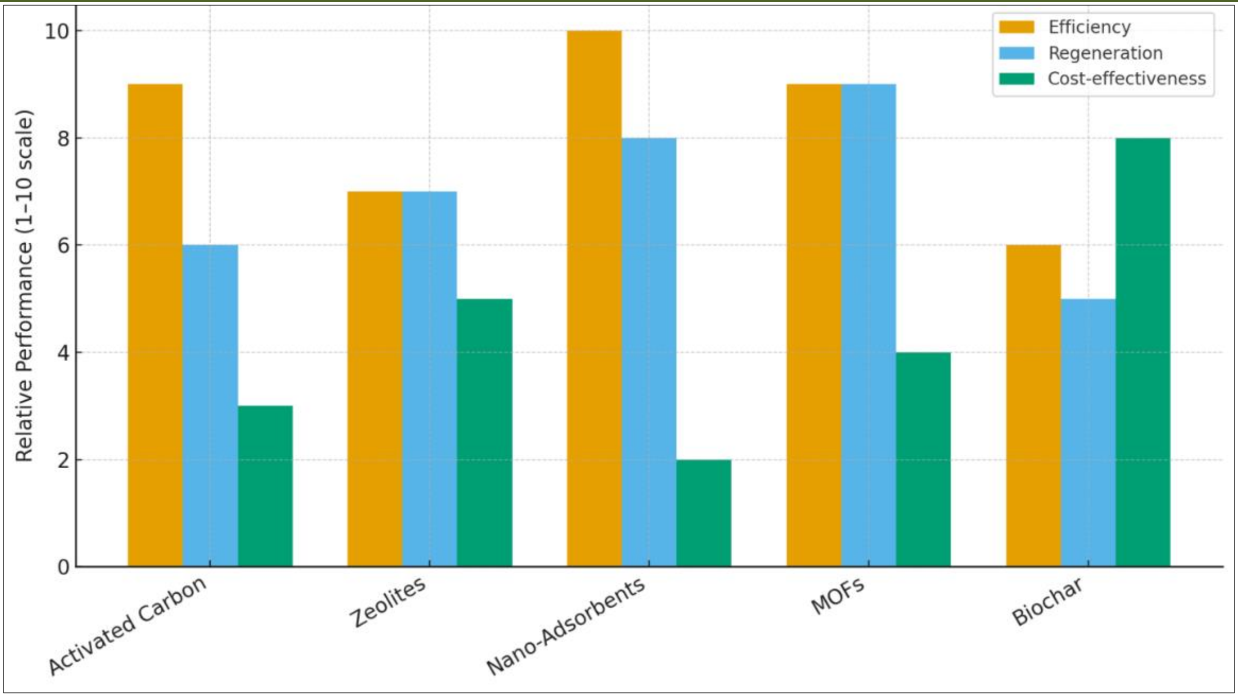
When compared to other treatment strategies, adsorption demonstrates unique advantages. Biological methods are generally effective for organic pollutants but less capable of removing heavy metals and inorganic compounds. Chemical oxidation can degrade a broad range of contaminants but often relies on harsh chemicals. Membrane filtration provides high removal efficiency but tends to be energy-intensive and expensive. In contrast, adsorption-based methods offer a flexible and frequently more cost-effective solution for addressing diverse pollutants [130].

Among conventional adsorbents, activated carbon is particularly effective in eliminating organic compounds, chlorinated species, and heavy metals. Its high-performance stems from its extensive surface area and porous structure. Nevertheless, its production is energy-intensive, and its efficiency may decline over time, requiring regeneration or replacement [41]. Zeolites are also widely used and are effective at removing cations such as heavy metals through ion exchange processes enabled by their crystalline framework. Although less energy-intensive to synthesize than activated carbon, their efficiency depends strongly on the specific zeolite type and the target pollutant [42].

Nano-adsorbents, especially those derived from carbon nanotubes and metal oxides, have emerged as highly promising candidates due to their high reactivity and large surface area. These materials excel in removing trace levels of both organic and inorganic contaminants. However, their synthesis can be complex and costly, and questions remain regarding their stability and environmental safety [131]. MOFs are another class of advanced adsorbents gaining attention for their exceptional porosity and structural tunability. Composed of metal clusters or ions coordinated with organic ligands, MOFs form crystalline frameworks with large surface areas that allow adsorption of a wide spectrum of pollutants, including pharmaceuticals and other emerging contaminants. Although MOF production can be energy-intensive, their impressive adsorption performance and ability to be regenerated with minimal loss of efficiency make them economically promising. Still, their long-term stability in aqueous environments and potential ecological impacts require further investigation [44].

Biochar, produced via biomass pyrolysis, is increasingly recognized for its sustainability and cost-effectiveness. It is particularly efficient in adsorbing heavy metals and organic pollutants, and its synthesis from agricultural residues makes it an attractive low-cost option. However, its adsorption performance is typically lower than that of activated carbon [12,132].

From an economic standpoint, the costs associated with adsorbent production and operation vary widely. Activated carbon offers high efficiency but at relatively high production costs. Biochar represents a low-cost alternative, though with somewhat lower efficiency. Nano-adsorbents, MOFs, and zeolites often entail higher costs due to complex synthesis requirements, yet their superior adsorption efficiency can justify the investment for specific applications.




**Graph 1: Comparative Performance of Key Adsorbents in Water Remediation**

The figure compares activated carbon, zeolites, nano-adsorbents, MOFs, and biochar across three parameters: pollutant removal efficiency, regeneration potential, and cost-effectiveness. It highlights the superior performance of advanced materials like nano-adsorbents and MOFs, while also recognizing biochar as a sustainable low-cost option.

### 7.3. Cost and Environmental Impact Analysis

The cost of preparing and applying adsorbents plays a crucial role in determining the feasibility of adsorption-based wastewater treatment, particularly when compared with other available technologies. A comprehensive cost evaluation may include raw material expenses, cost indices, discounted cash flow, and performance-based measures such as cost per gram of adsorbate removed, as well as annual capital expenditure (CAPEX) and operating expenditure (OPEX). Such assessments are critical for analyzing economic viability and determining the scalability of adsorbents from pilot to industrial levels [133].

Adsorption remains one of the most versatile, simple, and eco-friendly methods for pollutant removal, with additional benefits such as reusability and relatively low cost. Different adsorbent classes—including biochar, biosorbents, activated carbon, minerals, clays, nanoparticles, polymers, and composites—have demonstrated effectiveness in eliminating a wide range of contaminants from wastewater. However, these materials differ significantly in terms of accessibility, economic feasibility, regenerative potential, and environmental sustainability. Reducing costs while maintaining treatment efficiency continues to be a major goal in adsorption research.

To enable standardized evaluation, a cost-performance metric ($\hat{C}$), expressed in \$/mol, has been introduced. This metric is calculated by converting reported adsorption capacity into mol/g, cost into \$/g, and then determining the ratio. Most modern adsorbents fall within the range of 1–200 \$/mol, with values below 1 \$/mol considered very inexpensive and those above 200 \$/mol categorized as costly. Nevertheless, comparisons across adsorbent types must be made cautiously, as synthesis complexity and solution chemistry can influence outcomes [32].

In addition to cost, environmental impacts are a critical factor in adsorbent evaluation. The production, use, and disposal of adsorbents can have varying ecological consequences. For instance, adsorbents derived from waste materials provide both economic benefits and sustainability advantages by promoting resource recovery and minimizing waste. In contrast, adsorbents that require chemical activation or complex synthesis may contribute to environmental burdens through high energy consumption or chemical pollution. The disposal of spent adsorbents also poses risks of secondary contamination, especially when saturated with hazardous pollutants. Thus, balancing affordability with environmental safety is essential for advancing sustainable wastewater treatment [33,37,38].

**Table 7: Cost and Environmental Impact of Common Adsorbents**

| Adsorbent Type | Cost Level | Environmental Impact | Sustainability Aspects |
|---|---|---|---|
| Activated Carbon | Moderate to High | Energy-intensive production; risk from disposal | High efficiency; regenerable but costly |
| Zeolites / Clays | Low to Moderate | Lower synthesis energy demand; stable disposal | Naturally abundant; selective ion exchange |
| Biochar / Biosorbents | Low | Minimal environmental burden; made from waste biomass | Sustainable, low-cost, supports waste valorization |
| Nanoparticles | High | Potential toxicity; high synthesis energy | High efficiency, but concerns on long-term safety |
| MOFs | High | Complex synthesis, high energy demand; possible leaching | Excellent capacity; regenerable with efficiency |
| Polymer/Composites | Moderate to High | May release microplastics if not managed properly | Tunable properties; recyclable with modifications |

## 8. Future Prospects

Adsorption technologies for wastewater remediation are expected to undergo substantial advancements, driven by continuous research and innovation in material science and environmental engineering. The transition from traditional techniques, such as those based on activated carbon and zeolites, to advanced methods involving carbon nanotubes, MOFs, and graphene-based materials illustrates the rapid progress of the field. This shift underscores the ongoing balance between efficacy, cost-effectiveness, environmental sustainability, and practical feasibility. Looking ahead, adsorption research will continue to focus on developing high-performance, eco-friendly, and economically viable adsorbents. The following subsection outlines emerging trends and future directions that are likely to shape the next generation of adsorption technologies in wastewater treatment.

### 8.1. Predicted Trends in Wastewater Remediation

Wastewater remediation is a rapidly evolving field, with a wide range of methods developed to address diverse pollutants. These techniques span physical, chemical, biological, and physico-chemical processes, each offering distinct mechanisms and applications. Physical methods, such as filtration, sedimentation, and flotation, rely on the inherent properties of pollutants to separate them from wastewater. These approaches are simple and effective for specific types of contaminants [130].

Chemical methods, by contrast, utilize agents such as coagulants, flocculants, oxidants, and reductants to alter pollutant chemistry and facilitate removal. Within this category, Advanced Oxidation Processes (AOPs) are particularly notable, as they generate highly reactive oxygen species, such as hydroxyl radicals, capable of degrading persistent organic pollutants and neutralizing pathogenic microorganisms. AOPs include techniques such as Fenton and photo-Fenton reactions, ozonation, photocatalysis, and electrochemical oxidation, which may be applied in both homogeneous and heterogeneous forms [134–136].

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In the realm of biological methods, enzymatic treatments represent a promising innovation. These approaches use enzymes as biocatalysts to selectively degrade pollutants, with performance often enhanced by immobilization on substrates like membranes, beads, or nanomaterials [137]. Enzymes such as laccase, peroxidase, nitrilase, and lipase have proven particularly effective in breaking down complex contaminants [138]. Alongside these, bioremediation methods continue to advance, employing microorganisms or plants in strategies such as bioaugmentation, biostimulation, and phytoremediation, all of which demonstrate significant potential [139,140].

Among the available physico-chemical methods, adsorption stands out for its versatility and efficiency. This process operates by binding pollutants to the surface of adsorbents with high affinity and selectivity. A wide array of adsorbents—including activated carbon, zeolites, clay minerals, biochar, MOFs, and graphene-based materials—has been employed successfully. Adsorption is recognized for its cost-effectiveness, operational simplicity, and ability to remove pollutants ranging from heavy metals and dyes to oils and micropollutants. Its promise is particularly evident in tackling emerging contaminants such as pharmaceuticals, personal care products, and endocrine-disrupting compounds. These pollutants, although often present in trace concentrations, pose serious ecological and human health risks, and adsorption offers a highly selective method for their removal. Furthermore, adsorption can be integrated with other technologies, such as biodegradation and advanced oxidation, to form hybrid systems with enhanced efficiency [47,125,141].

Adsorption efficiency depends on parameters related to the adsorbent, the contaminant, and the wastewater matrix. Optimizing these parameters is vital for effective treatment, and this is increasingly supported by data-driven methods such as machine learning (ML) and artificial intelligence (AI). These tools reveal hidden patterns within complex datasets, predict performance under variable conditions, and provide insights into adsorption mechanisms. They also assist in adsorbent design, preparation, and process optimization. AI and ML are equally valuable for real-time monitoring, control, and diagnostics, improving the reliability of treatment systems. Advanced approaches such as artificial neural networks can even simulate adsorption at the molecular level, shedding light on surface interactions and pore diffusion dynamics [142].

The integration of nanotechnology, advanced materials, and AI-driven tools points toward a promising future for adsorption-based wastewater treatment. These developments pave the way for intelligent, sustainable systems capable of addressing both conventional and emerging pollutants. Nevertheless, challenges remain, including high computational demands, data availability, and model interpretability. Addressing these issues will require collaborative efforts among material scientists, engineers, and data scientists. The potential benefits, in terms of clean water availability and improved environmental health, are substantial and transformative.

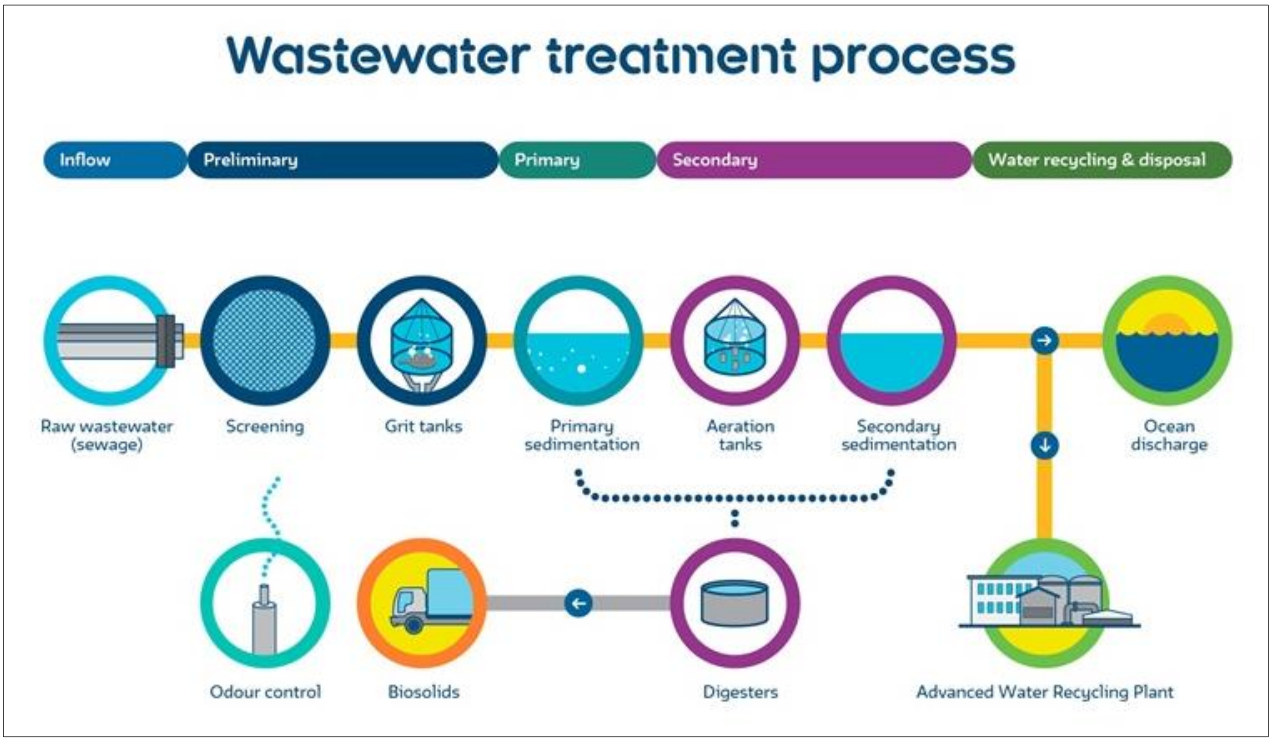


**Figure 5: Emerging Trends and Integrated Approaches in Wastewater Remediation**

Figure 5 illustrates the major predicted trends in wastewater treatment, spanning physical, chemical, biological, and physico-chemical processes. It highlights conventional stages (screening, sedimentation, biological treatment) alongside advanced chemical routes (AOPs) and hybrid adsorption–membrane schemes. Biological innovations (enzymatic and microbe-driven) and versatile adsorption using MOFs, graphene, and biochar are emphasized. Integration into hybrid systems shows how adsorption couples with biodegradation or oxidation for higher performance. Finally, AI/ML workflows signal a shift toward intelligent, adaptive treatment systems.

### 8.2. Potential Breakthroughs in Adsorption Technologies

The future of adsorption technology promises transformative advances for water purification and environmental sustainability. Several potential breakthroughs are anticipated, as outlined below and illustrated in *Figure 5*.

#### 8.2.1. Development of Highly Selective and Efficient Adsorbents

Researchers are actively developing new materials and modifying existing ones to improve selectivity and adsorption capacity for specific pollutants. This includes synthesizing nanostructured materials with high surface-to-volume ratios, providing increased contact areas for pollutant capture. Functionalization with tailored surface groups enables specific binding sites, while biomolecule incorporation—using enzymes or antibodies—leverages molecular recognition to selectively target contaminants [22].

#### 8.2.2. Incorporation of Advanced Materials

Advanced adsorbents such as carbon nanotubes, graphene, MOFs, and COFs are at the forefront of performance improvement. Carbon nanotubes and graphene, with their unique electrical, thermal, and mechanical properties, enhance both adsorption efficiency and selectivity. MOFs, with their tunable pore networks and functional groups, allow targeted pollutant capture [14,15,64]. More recently, COFs have gained attention due to their stability, large surface area, and adjustable pore sizes. Using dynamic covalent chemistry (DCC) and keto–enol tautomerism in COF synthesis introduces environmentally friendly frameworks for water remediation. Water itself is increasingly seen as a green solvent in these processes, further promoting sustainability [143,144].

#### 8.2.3. Design of Integrated Adsorption Systems

Combining adsorption with other treatment methods, including membrane filtration, photocatalysis, and biodegradation, can yield synergistic benefits. Membrane integration addresses large particles while adsorption captures dissolved pollutants. Photocatalysis complements adsorption by degrading organic contaminants. These integrated approaches also improve regeneration efficiency and reduce waste, offering more sustainable treatment options [70].

#### 8.2.4. Application of Machine Learning and Artificial Intelligence

Data analytics, ML, and AI are increasingly important in optimizing adsorption. These tools predict pollutant removal efficiencies, identify trends, and guide adsorbent preparation. AI systems also support real-time monitoring and adaptive control, ensuring high performance under variable water conditions [142]. A detailed discussion of ML and AI applications in adsorption is provided in Section 6.5.

#### 8.2.5. Development of Sustainable and Cost-Effective Adsorbents

Creating adsorbents from renewable or waste materials—such as biomass, agricultural residues, or industrial byproducts—can lower costs while reducing environmental impacts. Such approaches transform waste into valuable resources, aligning with circular economy principles and advancing resource efficiency [2,32].

#### 8.2.6. In-Situ Remediation and Point-of-Use Systems

Emerging work focuses on in-situ remediation at contamination sites, minimizing environmental disturbance and transport needs. In parallel, point-of-use systems are being developed for decentralized treatment in resource-limited areas, providing affordable access to clean water [145].

#### 8.2.7. Tailoring Adsorbents for Emerging Pollutants

Specialized adsorbents are being designed to target emerging contaminants such as pharmaceuticals, personal care products, and microplastics. These pollutants, often overlooked in conventional systems, require customized materials to address their diverse structures and behaviors [47].

#### 8.2.8. Regeneration and Reuse of Adsorbents

Improving adsorbent regeneration is critical for reducing waste and operational costs. Current research emphasizes eco-friendly, energy-efficient regeneration strategies to maintain adsorption performance while minimizing environmental impact [26].

#### 8.2.9. Understanding Adsorption Mechanisms at the Molecular Level

Greater insight into adsorption at the atomic scale can enable the design of materials with precisely tailored properties. Studying pollutant–surface interactions helps clarify the influence of pore size, surface chemistry, and material morphology on adsorption efficiency [146].

#### 8.2.10. Integration with Circular Economy Principles

Incorporating adsorption technologies into circular economy frameworks supports both pollutant removal and recovery of valuable resources, such as nutrients and metals. This dual benefit turns wastewater into a resource stream, promoting sustainability and reducing environmental footprints [147].

### 8.3. Implications for Sustainability and Environmental Health

When aligned with green chemistry principles, advanced adsorption technologies offer immense potential to improve both environmental health and sustainability. The development of "green" adsorbents using waste or renewable raw materials reduces ecological impacts and carbon emissions throughout their lifecycle. Biochar derived from agricultural or forestry residues exemplifies this dual benefit, effectively removing contaminants while contributing to resource recovery. Large-scale deployment of optimized adsorption technologies, particularly when powered by renewable energy, could significantly expand access to clean water while safeguarding aquatic ecosystems worldwide [148].

Nonetheless, nanoscale adsorbents raise toxicity concerns that must be carefully addressed to ensure benefits outweigh risks. Standardized life cycle assessment frameworks, including toxicity evaluations, are needed to guide responsible design and application. Emerging research suggests that green synthesis pathways—such as using plant extracts—can reduce cytotoxicity and ecological risks associated with nano-adsorbents. However, further study and development are required to unlock the full potential of green engineered adsorbents for safe and sustainable water remediation [148,149].

With responsible innovation and governance, adsorption technologies that embrace sustainability principles hold great promise for ensuring cleaner water resources for both present and future generations.

## 9. CONCLUSION

Advances in nanotechnology and materials science have greatly enhanced the efficiency, selectivity, and stability of adsorption, positioning it as a leading strategy for advanced water purification. Yet, despite these scientific breakthroughs, challenges remain in scaling laboratory innovations into cost-effective, real-world applications. Artificial intelligence (AI) and machine learning (ML) present powerful tools to bridge this gap by optimizing adsorption processes, improving material design, and enhancing predictive capabilities under diverse environmental conditions.

Future research should emphasize the development of sustainable, eco-friendly adsorbents through green synthesis routes, alongside economically viable production methods. Standardized evaluation frameworks that assess both environmental and economic impacts are critical for ensuring long-term feasibility and sustainability. Interdisciplinary collaboration between material scientists, environmental engineers, data scientists, and policymakers will be essential to translate these innovations into scalable, practical solutions.

By combining novel materials with data-driven optimization approaches, adsorption-based technologies can deliver efficient, affordable, and sustainable wastewater treatment solutions—contributing meaningfully to global efforts toward clean water access and environmental protection.

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