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Innovations and challenges in adsorption-based wastewater remediation: A comprehensive review

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ABSTRACT

Water contamination is an escalating emergency confronting communities worldwide. While traditional adsorbents have laid the groundwork for effective water purification, their selectivity, capacity, and sustainability limitations have driven the search for more advanced solutions. Despite many technological advancements, economic, environmental, and regulatory hurdles challenge the practical application of advanced adsorption techniques in large-scale water treatment. Integrating nanotechnology, advanced material fabrication techniques, and data-driven design enabled by artificial intelligence (AI) and machine learning (ML) have led to a new generation of optimized, high-performance adsorbents. These advanced materials leverage properties like high surface area, tailored pore structures, and functionalized surfaces to capture diverse water contaminants efficiently. With a focus on sustainability and effectiveness, this review highlights the transformative potential of these advanced materials in setting new benchmarks for water purification technologies. This article delivers an in-depth exploration of the current landscape and future directions of adsorbent technology for water remediation, advocating for a multidisciplinary approach to overcome existing barriers in large-scale water treatment applications.

1. Introduction

Wastewater management remains the utmost challenge toward environmental sustainability and public health. Among numerous techniques developed for the treatment of wastewater, adsorption has been found to be one of the most effective and versatile methods due to its simplicity, efficiency, and the broad range of pollutants it can remove. Activated carbon, made from natural materials, has been crucial for cleaning water since the early 20th century because it can remove numerous types of pollutants. However, the search for better, cheaper, and more eco-friendly cleaning materials continues. This is because wastewater is getting more complicated and environmental laws are becoming stricter, pushing for new and improved methods beyond the usual ones [1]. The advent of nanotechnology marks a significant change in the development of materials used for adsorbent development. This technology allows for the manipulation of materials at a molecular scale, leading to higher efficiency in capturing pollutants. Innovations such as carbon nanotubes, graphene, metal-organic frameworks (MOFs), and nanostructured polymers are at the forefront, offering better performance, specificity, and reusability than older methods. These nanoscale materials demonstrate the possibility of precisely removing specific pollutants, such as heavy metals, organic compounds, and new threats like drugs and hormone disruptors, establishing a new standard for water purification technology [2].

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The arrival of AI and ML in adsorption science marks a major breakthrough. These powerful tools offer solutions to long-standing challenges, like improving regeneration efficiency and predicting how adsorption behaves under changing environmental conditions. By leveraging artificial intelligence (AI) and machine learning (ML), scientists can now tailor materials and processes, leading to smarter adsorbents that adapt to their environment. This not only enhances the effectiveness and eco-friendliness of adsorption methods but also unlocks new possibilities for tackling intricate wastewater treatment problems. Alongside these technological advancements, analytical techniques like scanning electron microscopy (SEM) and high-performance liquid chromatography (HPLC) are making significant progress. These tools provide valuable information on the physical and chemical interactions between adsorbents and pollutants, offering a deeper understanding of the factors that influence the adsorption process. This newfound knowledge paves the way for optimizing this crucial technology [3–5].

The shift towards low-carbon solutions, with a strong focus on energy conservation and resource recycling, has presented new challenges to traditional wastewater treatment methods [6]. While advancements are promising, implementing these advanced adsorption techniques in large-scale wastewater treatment faces hurdles. Scaling up the process, managing the cost, and ensuring the environmental safety of both the production and disposal of the adsorbents are major concerns [7]. Additionally, potential risks posed by nanomaterials to the environment and human health need careful consideration. Overcoming these challenges requires a unified effort from various fields, including material science, environmental engineering, toxicology, and regulatory bodies [8]. This review explores the recent advancements in materials science and nanotechnology, brought to reality by AI and ML, which are pushing adsorption techniques forward. This review also explores how these innovations could impact costs and the environment, as well as the future trends in cleaning wastewater. By simplifying complex technologies and their implications, we tried to shed light on how these advancements can lead to more sustainable and efficient ways to ensure clean water, reflecting on the broader significance of environmental health and sustainability.

2. Historical analysis of adsorption techniques

Adsorption is the phenomenon where molecules of an adsorbate substance attach to the surface of an adsorbent substance through intermolecular forces. Adsorption has been widely used as a wastewater treatment technique for removing contaminants from aqueous solutions, such as organic pollutants, heavy metals, dyes, nutrients, and pathogens [9]. The history of adsorption as a wastewater treatment technique can be traced back to the late 19th century, when the first activated carbon filter was patented by R. V. Ostrejko in 1900 [1]. Since then, activated carbon has been extensively used as an adsorbent for water purification due to its high surface area, porosity, and affinity for organic compounds. However, activated carbon also has some drawbacks, such as high cost, low selectivity, and difficulty in regeneration [10]. Therefore, researchers have explored other types of adsorbents, such as natural materials (e.g., clay, zeolite, biomass), synthetic materials (e.g., silica gel, metal oxides, polymers), and hybrid materials (e.g., metal-organic frameworks, carbon nanotubes, graphene oxide), for wastewater treatment. These adsorbents have different characteristics and advantages over activated carbon, such as higher adsorption capacity, selectivity, stability, recyclability, and lower cost. The development of adsorption techniques for wastewater treatment has been driven by the increasing demand for clean water and stringent environmental regulations [11,12].

3. Notable progress in the last decade

Over the past ten years, substantial progress has been achieved in improving the adsorption capabilities and specificities of newly designed adsorbents, alongside a deeper comprehension of adsorption mechanisms and kinetics. One of the major breakthroughs in the fabrication of adsorbents is the application of nanotechnology, which allows the synthesis of nanoscale materials with unique properties, such as high surface area, tunable pore size and shape, and functional groups. Nanomaterials have the potential to serve as standalone adsorbents or as fundamental components in the construction of composite adsorbents. Some examples of nanomaterials that have been widely studied for adsorption purposes are carbon nanotubes, graphene, metal oxides, metal-organic frameworks, zeolites, and magnetic nanoparticles [13]. These nanomaterials can exhibit high adsorption capacities for various pollutants due to their large surface area and specific interactions with the pollutant molecules. For instance, carbon nanotubes can remove dyes and heavy metals from water by π-π stacking and electrostatic interactions, while metal-organic frameworks can selectively adsorb organic compounds and nutrients by coordination bonding and molecular sieving [14,15].

Another important aspect of adsorbent fabrication is the modification of natural or synthetic materials to improve their adsorption performance. Modification methods can include physical treatments, such as thermal activation, acid or base washing, and irradiation; chemical treatments, such as impregnation, grafting, and coating; and biological treatments, such as biosorption and biochar production. These methods can alter the surface properties of the adsorbents, such as surface area, porosity, charge, hydrophobicity, and functional groups [16]. The development of novel adsorbents and modification methods has been accompanied by the advancement of analytical techniques and theoretical models that can help elucidate the adsorption mechanisms and kinetics. Analytical techniques can provide information on the physicochemical characteristics of the adsorbents and the pollutant molecules, such as surface morphology, elemental composition, functional groups, pore size distribution, surface charge, molecular structure, and solubility. Some examples of analytical techniques that have been widely used for adsorption studies are SEM, transmission electron microscopy (TEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), Fourier transform infrared spectroscopy (FTIR), nuclear magnetic resonance (NMR), thermogravimetric analysis (TGA), Brunauer-Emmett-Teller (BET) method, zeta potential measurement, ultraviolet–visible (UV–Vis) spectroscopy, and HPLC. These techniques can help identify the main factors that affect the adsorption process, such as surface area, pore size, surface charge, functional groups, molecular size, polarity, and pH [5]. Fig. 1 illustrates the primary categories of adsorbents, detailing their essential properties and the methodologies employed for their respective characterization.

Theoretical models can help describe the adsorption process mathematically and predict the adsorption behavior under different conditions. Theoretical models can be categorized into two groups: equilibrium models and kinetic models. Equilibrium models can illustrate the correlation between the quantity of pollutant adsorbed onto the adsorbent surface and the equilibrium concentration of the pollutant within the solution. Some examples of equilibrium models are the Langmuir model, Freundlich model, Temkin model, and Dubinin-Radushkevich model. These models can furnish data regarding the highest achievable adsorption capacity, the strength of adsorption, the heat involved in adsorption, and the nature of adsorption (isotherm). Kinetic models can explain the speed at which pollutant adsorption occurs on the adsorbent surface, including the various factors that affect this process, such as mass transfer, diffusion, and reaction. Some examples of kinetic models are pseudo-first-order model, pseudo-second-order model, intraparticle diffusion model, and Elovich model. These models can provide information on the rate constant, the equilibrium amount, the diffusion coefficient, and the activation energy of adsorption [17].

4. Detailed analysis of current limitations

Despite the remarkable progress in the development of adsorption techniques for wastewater treatment, there are still some challenges and limitations that need to be addressed. These limitations can be classified into six categories: adsorption capacity, selectivity and non-specific binding, material degradation and stability, recovery and reusability of adsorbents, economic viability, and regulatory and environmental challenges. Each of these categories is discussed in detail in the following subsections.

4.1. Adsorption capacity

Adsorption capacity determines the efficiency and effectiveness of adsorption techniques for wastewater treatment. Adsorption capacity refers to the quantity of adsorbate that a given mass of adsorbent can capture in specific conditions. The capacity for adsorption is influenced by a range of factors (Table 1), including attributes of the adsorbent (like surface area, porosity, and functional groups), properties of the adsorbate (such as molecular size, polarity, and concentration), and the conditions under which the adsorption occurs (including temperature, pH, and contact time) [2,18]. One of the current limitations of adsorption techniques is that the adsorption capacity of most adsorbents is still relatively low compared to the high concentration and diversity of contaminants in wastewater. A significant quantity of adsorbent is necessary to attain effective removal rates, leading to heightened expenses and intricacy in the treatment procedure. Moreover, the adsorption capacity of most adsorbents tends to decrease with increasing initial concentration of adsorbate, due to the saturation of available binding sites on the adsorbent surface [19]. Therefore, there is a need to develop novel adsorbents with higher adsorption capacity and affinity for various contaminants in wastewater.

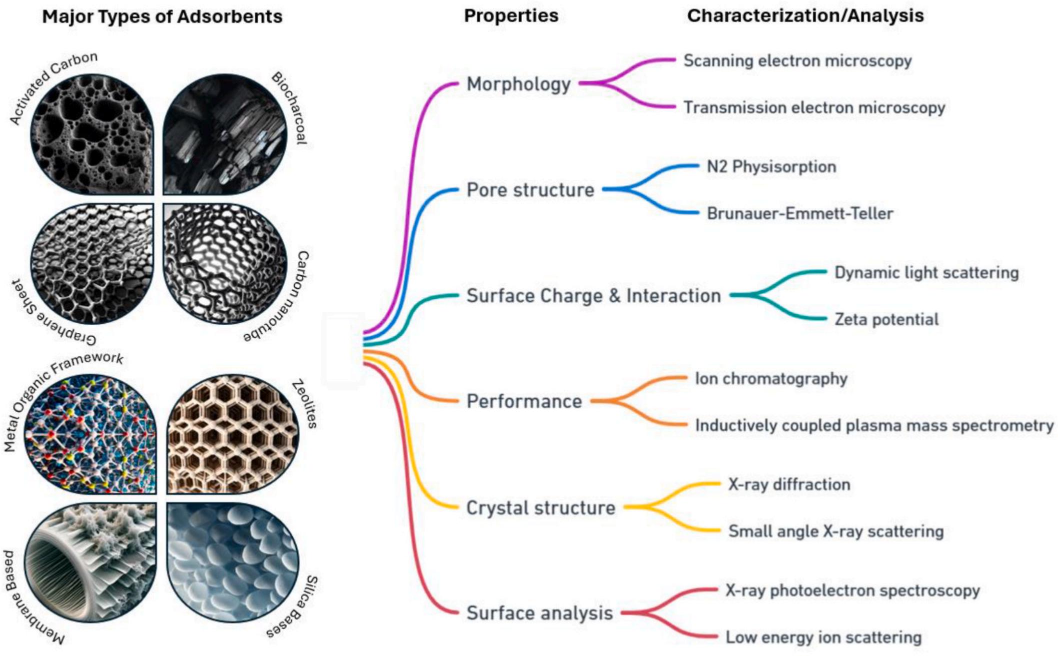

Fig. 1. Key adsorbent types, their properties and techniques used for respective characterization.

Table 1
Factors affecting adsorption capacity and their effects.

Factor	Effect
Surface area	Enhances capacity by providing more adsorption sites.
Porosity	Increases capacity by offering additional space for molecules.
Functional groups	Enhance capacity through specific interactions with target molecules.
Molecular size	Smaller molecules are adsorbed more effectively due to better access.
Polarity	Capacity increases for polar molecules on polar adsorbents.
Concentration	Higher concentrations lead to greater capacity until saturation.
Temperature	Higher temperatures can enhance capacity, but effects vary.
pH	Affects adsorbent charge and target molecule ionization, impacting capacity.

4.2. Selectivity and non-specific binding

The performance and suitability of adsorption techniques for wastewater treatment depend significantly on their selectivity. It pertains to an adsorbent material's capacity to specifically adsorb and retain a desired adsorbate from a mixture of different substances present in water. The selectivity of an adsorbent depends on several aspects, such as the surface chemistry, the pore size distribution, and the functional groups of the adsorbent, as well as the molecular size, shape, polarity, and charge of the adsorbates. Furthermore, the selectivity of the adsorbent is also influenced by operating parameters like temperature, pH, and ionic strength [20]. However, achieving high selectivity is a challenging task, especially when dealing with the complex and diverse contaminants present in wastewater. For instance, activated carbon, a common adsorbent material, can remove a wide range of organic pollutants from water through various interactions, such as hydrophobic, π–π stacking, hydrogen bonding, and electrostatic interactions. However, these interactions also make activated carbon attract water molecules and other polar compounds, which reduces its selectivity and specificity for organic pollutants in wastewater [21]. Another challenge in adsorption technology is the competitive adsorption effect, which occurs when different adsorbate species compete for the limited surface sites of the adsorbent. As the initial concentration of adsorbates in water increases, the competition among them also intensifies, resulting in lower selectivity. This effect is a practical issue that requires careful optimization of the operating conditions and the selection of the adsorbent material to achieve a balance between selectivity and efficiency [22]. Fig. 2 Illustrates the critical factors that influence the selectivity of adsorbents for wastewater remediation.

4.3. Material degradation and stability

Material degradation and stability are defined as the ability of an adsorbent to maintain its structure, function, and performance under various environmental and operational conditions [23]. Material degradation and stability depend on various factors, such as the characteristics of the adsorbent (e.g., chemical composition, crystallinity, morphology), the properties of the adsorbate (e.g., acidity, redox potential, biodegradability), and the operating conditions (e.g., temperature, pH, contact time) [24]. One of the current limitations of adsorption techniques is that the material degradation and stability of most adsorbents are still relatively low compared to the harsh and complex conditions of wastewater. Moreover, the material degradation and stability of most adsorbents tend to decrease with increasing contact time or repeated use, due to the physical or chemical deterioration of the adsorbent surface or

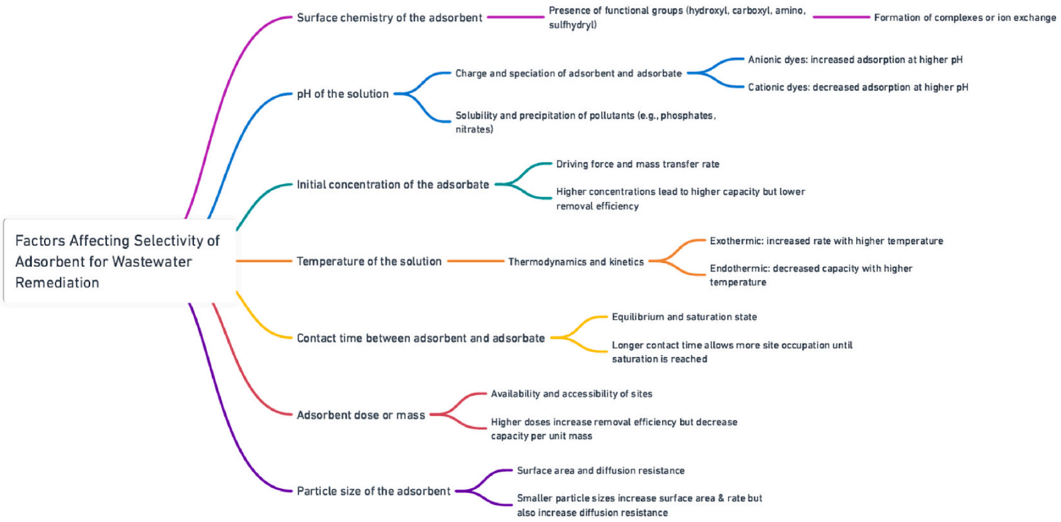

Fig. 2. Factors affecting selectivity of adsorbent for wastewater remediation.

structure [25]. Table 2 provides a comprehensive overview of the elements that impact the degradation and durability of typical adsorbents employed for wastewater treatment.

4.4. Recovery and reusability of adsorbents

Recovery and reusability of adsorbents are defined as the ability of an adsorbent to be separated from the treated water and to be reused for subsequent adsorption cycles after regeneration. Recovery and reusability of adsorbents depend on various factors, such as the characteristics of the adsorbent (e.g., density, magnetic property, shape, size), the properties of the adsorbate (e.g., solubility, biodegradability, toxicity), and the operating conditions (e.g., temperature, pH, contact time) [26]. One of the present constraints of adsorption methods is that, in comparison to the extensive use and frequent treatment of wastewater, the ability to recover and reuse the majority of adsorbents remains relatively limited. Moreover, the recovery and reusability of most adsorbents tend to decrease due to fouling of the adsorbent surface or pores by organic matter or inorganic precipitates [23]. Magnetic adsorbents overcome some limitations regarding reusability by allowing easy separation through the application of an external magnetic field, thereby reducing energy consumption, and minimizing adsorbent loss during the recovery process. Moreover, they have demonstrated high adsorption performance for various micropollutants, including heavy metals, dyes, pharmaceuticals, pesticides, and organic compounds [27]. However, some challenges need to be overcome for the practical application of magnetic adsorbents in wastewater treatment. These include the stability of the magnetic adsorbent under different environmental conditions, such as pH, temperature, salinity, and redox potential, which may affect the magnetic property and the adsorption capacity of the adsorbent [28]; the regeneration methods of the magnetic adsorbent, which may influence the recovery and reusability of the adsorbent [29]; and the ecotoxicological impact of the magnetic adsorbent, which may pose potential risks to the aquatic ecosystems and human health [30,31]. Fig. 3 Illustrates the key challenges in magnetic adsorption technology, including stability, synthesis, regeneration, and ecotoxicological limitations.

4.5. Economic viability

The widespread acceptance and long-term sustainability of adsorbents in wastewater treatment are heavily dependent on their economic feasibility. Despite the numerous advantages offered by adsorption, including its simplicity, efficiency, and selectivity compared to conventional treatment approaches, economic viability remains a significant obstacle. The cost of adsorbents is significantly influenced by their source, production method, and surface properties. Activated carbon, a commonly used adsorbent, is relatively expensive due to its energy-intensive production process. Economical and promising solutions are provided by alternative adsorbents sourced from agricultural or industrial waste materials like chitosan, zeolites, and activated clay [2,32]. The properties of the wastewater, including pollutant concentration, diversity, and toxicity, also impact the economic viability of adsorption. Highly concentrated or diverse wastewater streams may require higher adsorbent dosages, increasing treatment costs. Additionally, the presence of toxic pollutants can necessitate regeneration or disposal of spent adsorbents, further adding to the economic burden [2].

4.6. Regulatory and environmental challenges

One of the current limitations of adsorption techniques for wastewater treatment is the regulatory and environmental challenges associated with the use, disposal, and management of adsorbents. The regulatory challenges include the lack of clear and consistent standards and guidelines for the quality, performance, and safety of adsorbents, as well as the compliance and monitoring of their application in wastewater treatment [33]. Different countries and regions may have different regulations and requirements for the approval, certification, and testing of adsorbents, which may pose difficulties and uncertainties for the manufacturers, suppliers, and users of adsorbents. Moreover, regulatory challenges may also affect the innovation and development of novel adsorbents, as the approval process may be lengthy, costly, and complex. Therefore, there is a need to harmonize and streamline the regulatory framework for adsorbents at the national and international levels, as well as to promote the awareness and education of the stakeholders on the benefits and risks of adsorbents [34,35]. The environmental challenges include the potential impacts of adsorbents on human health and the environment during their production, use, disposal, and recycling. The production of adsorbents may involve

Table 2
Fundamental challenges and recent breakthroughs related to improving the stability of adsorbent materials used in water remediation.

Adsorbent	Challenges	Advancements	Reference
Activated Carbon	Surface oxidation, functional group loss, pore collapse	Surface modification, templating synthesis	[10,56]
MOFs	Structural collapse, linker degradation, thermal stability	Designer linkers, post-synthetic modifications, dual passive heat dissipation approach	[57,58]
Zeolites	Dealumination, lattice collapse	Hydrothermal stabilization, silylation	[42,43]
Polymer Resins	Physical aging, swelling, chain scission	Crosslinking, imprinting	[59]
Biosorbents	Biodegradation, pore blockage	Chemical modification, immobilization	[38,60]
Silica Gels	Dissolution in high-pH environments	Surface modification, composite formation	[61]
Alumina	Loss of porosity and surface area	Sol-gel synthesis, doping	[62]
CNTs	Oxidation, loss of walls/layers	Functionalization, encapsulation	[63]
Graphene Oxide	Loss of functional groups, restacking	Reduction methods, composite formation	[64]

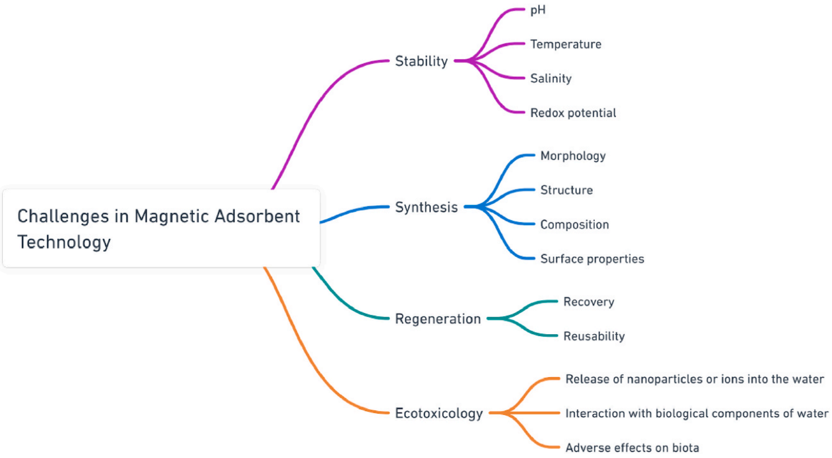

Fig. 3. Key challenges in magnetic adsorption technology.

the consumption of energy and resources, as well as the generation of emissions and wastes [36]. The use of adsorbents may introduce new contaminants or alter the physicochemical properties of wastewater, which may affect the downstream processes or receiving water bodies. The disposal of adsorbents may pose risks of leaching, migration, or bioaccumulation of pollutants in soil, water, or biota. The recycling of adsorbents may require additional treatments or processes that may have environmental implications. Hence, it is imperative to evaluate and reduce the environmental consequences of adsorbents throughout their entire life cycle and embrace the principles of eco-friendly chemistry and engineering in their design and development [37,38].

5. Advances to overcome current limitations

While substantial advancements have been made in creating innovative adsorbents for water purification, certain limitations persist and demand attention to elevate both their performance and applicability. **Section 4** outlines these limitations, and the subsequent sub-section below explores recent breakthroughs aimed at overcoming these challenges. Additionally, it outlines future directions for further enhancements in this domain.

5.1. Adsorption capacity

In recent studies, there has been a strong emphasis on developing novel adsorbents to enhance the adsorption capacity for contaminant removal from wastewater. One major advancement is utilizing nanostructured materials like carbon nanotubes (CNT), MOF and graphene which possess extremely high surface areas, improving binding sites for adsorbate molecules. Tailoring the pore sizes in mesoporous and micro/mesoporous hierarchical structures has further enhanced size-exclusion effects, allowing for selective contaminant capture. The unique properties of these nanostructured materials are not limited to their surface area. They also facilitate specific chemical interactions and nanoconfinement effects, which significantly boost the adsorption process. The importance of these interactions cannot be overstated, as they provide new avenues for capturing and removing contaminants that were previously challenging to address [21,39]. In parallel with the development of new adsorbent materials, computational tools have emerged as a powerful ally in the field. These tools are used to screen a vast array of materials, including metal-organic frameworks (MOFs), to identify the most effective adsorbent candidates. MOFs, with their customizable structures and functionalities, have shown great promise in adsorption applications due to their high porosity and tunable chemical properties [40].

In water remediation, achieving consistent adsorption across wide range of physico-chemical stresses possesses a significant challenge. Fortunately, several material classes exhibit remarkable resilience in these scenarios. Activated carbon, with its large surface area and diverse functional groups, excels in adsorbing organic pollutants across a wide pH range [41]. Modified clays like zeolites boast tunable pore sizes and surface charges, enabling targeted adsorption of specific contaminants even amidst fluctuating pH [42,43]. MOFs offer exceptional versatility, with their customizable pore structures and metal centers allowing for selective adsorption of a broad spectrum of pollutants under varying temperatures and pH [44]. Additionally, biopolymer-based adsorbents derived from chitosan and cellulose exhibit strong pH stability and the ability to complex with heavy metals through natural functional groups [45,46]. By strategically choosing and modifying these robust materials, we can create efficient and adaptable adsorbents for tackling the dynamic complexities of water pollution.

Moreover, functionalization techniques have been developed to introduce specific functional groups onto the adsorbent materials. These functional groups are selected based on their ability to interact with various contaminants, whether they are polar/nonpolar organic or ionic inorganic. This approach allows for targeted removal of specific contaminants, enhancing the overall efficiency and selectivity of the adsorption process [47]. Recent research and developments in wastewater treatment techniques had made significant strides in developing novel adsorbents with tunable properties. These advancements are not only enhancing the efficiency of contaminant removal but also paving the way for more cost-effective and environmentally sustainable wastewater treatment solutions.

5.2. *Selectivity and non-specific binding*

In recent times, there have been notable developments aimed at addressing the challenges of selectivity and non-specific binding in adsorbents. This is an important aspect in the areas of chemical, environmental, and biological engineering. These innovations are focused on enhancing the specificity and efficiency of adsorbents through various approaches. One of the key developments in this area is the use of Molecularly Imprinted Polymers (MIPs). MIPs are engineered to replicate the molecular recognition found in natural systems. They are created with a template molecule, which is subsequently extracted, resulting in a cavity that matches the shape and functional groups of the intended molecule. This approach significantly improves the selectivity of the adsorbent by enabling it to recognize and selectively bind to specific molecules, reducing non-specific interactions [48]. The advancement in inorganic molecular imprints, such as those made on titanium dioxide or silica-titania composites, has also shown great promise. These inorganic moulds provide enhanced thermal and chemical resilience when compared to their organic equivalents. This stability is crucial for applications that involve extreme conditions, such as high temperatures or corrosive environments [49,50]. Another notable innovation is the development of single crystal surface molecular imprinting. This technique uses single crystals of metal oxides or metal-organic frameworks as the substrate for imprinting. The advantage of using single crystals lies in their flat and rigid surfaces, which lead to high-quality imprinting sites with reduced non-specific adsorption [51].

Hydrophilic-hydrophobic interactions have been exploited to improve the selectivity of adsorbents. By designing adsorbents with hydrophobic surfaces, it’s possible to preferentially adsorb hydrophobic molecules from hydrophilic environments. This principle has been effectively applied in environmental remediation, such as in the selective adsorption of oil spills [52].

Electrostatic interactions are another area of focus. Adsorbents can be engineered to selectively bind charged pollutants through electrostatic forces. This approach is particularly useful in water treatment processes, where it can be used to remove ionic dyes and other charged contaminants [53]. The surface acid-base interaction is also a key area of research. By modifying the surface chemistry of adsorbents to include acidic or basic functional groups, it’s possible to target specific pollutants that can participate in acid-base interactions. This method is effective for enriching pollutants that can accept or donate electrons or protons [54]. Finally, the regulation of redox species on the surface of adsorbents has been explored to enhance selectivity. By tailoring the redox properties, adsorbents can be designed to favour specific interactions with target molecules, thus improving selectivity and reducing non-specific binding [55]. The advancements discussed in this section represent a significant step forward in addressing the challenges of selectivity and non-specific binding in adsorbents. By incorporating principles from chemistry, materials science, and engineering, researchers have developed innovative solutions that hold great promise for a wide range of applications for water remediation.

5.3. *Material degradation and stability*

Adsorbents have been pivotal in removing pollutants from water, but their effectiveness is often hindered by operational stability and material degradation over time. The recent push in research has been towards the development of novel adsorbents with enhanced resistance to a broad spectrum of physico-chemical stresses. Activated carbon advancements include surface modifications that enhance resistance to oxidation and improve adsorption capacity. For MOFs, the development of designer linkers and hydrophobic functional groups has addressed concerns about structural collapse. Hydrothermal stabilization and silylation approaches can be used to prevent dealumination in zeolites, while polymer resins have gained durability through crosslinking and specialized contaminant targeting via imprinting techniques. Biosorbents have seen improved biodegradation resistance through chemical modification and immobilization strategies. Silica gels have been enhanced with organosilane grafting for better stability, and alumina’s thermal stability has been improved via sol-gel synthesis and doping. CNTs and Graphene Oxide can be enhanced through functionalization and reduction techniques, ensuring the preservation of their adsorption efficacy. Table 2 summaries the core challenges and recent advancements in enhancing the stability of adsorbent materials for water remediation, highlighting the multidisciplinary approach required to address the complexities of water treatment technologies.

5.4. *Recovery and reusability of adsorbents*

The widespread adoption of adsorbents is often hindered by the limitations associated with their recovery and reusability. Traditional methods including filtration, centrifugation, and sedimentation often suffer from inefficiency, high energy consumption, and/or a requirement of additional steps for further processing of the recovered adsorbent. Researchers are constantly developing new and improved methods to recover and reuse adsorbents, making the water treatment process both cheaper and more environmentally friendly.

A crucial challenge in reusability is maintaining the magnetic property over repeated use. This is addressed through covalent immobilization of biopolymers onto the particle’s surface. This method significantly strengthens the bond between the adsorbent and the biopolymer, minimizing leaching and remarkably preserving the adsorbent’s capacity to capture contaminants across multiple regeneration cycles [65]. By employing strategies like the in situ synthesis of magnetite nanoparticles within biopolymer matrices, researchers have successfully created adsorbents that exhibit superior performance in pollutant uptake and can be easily separated from treated water using magnets. These biosorbents have shown remarkable efficiency in the removal of a wide range of contaminants, from heavy metals to organic dyes, under various water treatment scenarios. The rational design of these materials focuses on optimizing the surface characteristics of the adsorbents to maximize their adsorption capacities and ensure their stability and reusability in successive treatment cycles [66]. Moreover, the integration of biopolymers such as chitosan, carrageenan, and cellulose into magnetic bio-nanocomposites has been extensively researched for their environmental compatibility and potential for biodegradability. These naturally derived materials offer the dual benefits of high adsorption efficiency and ecological safety, making them ideal candidates for sustainable water remediation technologies. The cross-linking of biopolymers with magnetic nanoparticles has been identified as a key technique for enhancing the mechanical strength and chemical stability of the adsorbents. thereby improving their performance and durability in practical applications. This strategy not only makes the biosorbents more resistant to harsh environmental conditions but also mitigates the risk of biopolymer release into the treated water [67]. Recent advancements in material science have led to the development of monolithic covalent organic frameworks (COFs) with hierarchical structures, notably in the form of COF-chitosan aerogels using a dual double-cross-linking approach. These aerogels, notable for their high porosity and low density, can float on water, making them easily recoverable and reusable for environmental remediation. This innovative approach has been successfully applied to remove 102.5 mg/g of sulfamerazine from water, showcasing its potential in water remediation [68,69].

Integrating adsorbent materials with membranes offers another exciting avenue for improved recovery and reusability. These membrane-based adsorbent technologies combine the advantages of adsorption with the ease of separation offered by membranes. One approach involves immobilizing the adsorbent material onto the membrane surface, allowing for direct contact with the contaminated water while enabling easy backwashing for regeneration. Alternatively, hollow fiber membranes can be filled with adsorbent particles, creating a contactor system where contaminated water flows through the fibres while the adsorbent remains confined. Both approaches demonstrate significant improvements in separation efficiency and facilitate the regeneration process, making them attractive options for large-scale water treatment applications [70,71].

5.5. *Economic and ethical challenges*

Efforts to address the economic and ethical issues related to adsorbents for water remediation have led to new scientific and technological advancements. These advancements focus on making these materials more effective, sustainable, and affordable. From a material science perspective, the economic viability of adsorbents is intricately linked to their synthesis and operational costs. Progress in green chemistry have led to the development of low-cost, high-performance adsorbents through the utilization of sustainable synthesis routes that minimize energy consumption and reduce the reliance on expensive or hazardous precursors.

Techniques such as sol-gel processes, hydrothermal synthesis, and bio-fabrication have been optimized to produce adsorbents with enhanced adsorption capacities and regeneration efficiencies. These methodologies not only address economic constraints but also align with ethical considerations by reducing the environmental impact associated with adsorbent production [72]. The ethical challenges in adsorbent application, particularly concerning lifecycle environmental impacts, have prompted the integration of circular economy principles into adsorbent development. The design of adsorbents now increasingly considers half-life scenarios, promoting the use of biodegradable materials or enabling the regeneration and reuse of adsorbents. This shift towards circularity is complemented by advancements in adsorbent modification techniques, such as surface functionalization and composite formation, which aim to extend the lifespan of adsorbents and enhance their performance in water remediation applications [73]. Technological innovations have also played a crucial role in addressing the limitations of adsorbents. The integration of adsorbent materials with advanced water treatment technologies, such as membrane filtration and photocatalytic degradation, has led to the development of hybrid systems that offer improved efficiency and selectivity in pollutant removal. These systems leverage the synergistic effects between adsorption processes and other treatment mechanisms, potentially lowering operational costs and mitigating the formation of secondary pollutants [74].

Additionally, the evaluation of adsorbents from both an economic and ethical perspective has been enhanced using sophisticated assessment techniques, including life cycle assessment (LCA) and cost-benefit analysis (CBA). These assessments provide a comprehensive framework for evaluating the sustainability and economic feasibility of adsorbent technologies, encompassing the entire spectrum from raw material acquisition through to disposal or regeneration. By quantifying the environmental impacts and economic costs associated with different adsorbent systems, these methodologies support informed decision-making in the selection and optimization of water remediation strategies [75]. Another important facet of recent studies is the employment of surrogate-based optimization strategies. This method balances cost-effectiveness with treatment efficacy, an essential element for practical implementation. These modelling techniques play a vital role in moving innovations from the research phase to market-ready solutions, thereby hastening the introduction of novel technologies in wastewater treatment [75].

6. Case studies of novel approaches

The field of water remediation has seen exciting advancements in adsorption technologies, offering new and effective ways to tackle different types of water pollution. These advancements include a variety of methods like biochar-based adsorbents, nanomaterials, metal-organic frameworks, and hybrid or composite adsorbents. There are also innovative techniques using membranes and the application of machine learning and AI to improve adsorption processes. The following subsections explore each of these innovative approaches, highlighting how they contribute to advancements in water purification.

6.1. *Biochar-based adsorbents*

The development of biochar-based adsorbents for water remediation has embraced a variety of innovative methods to improve pollutant removal efficiency. These advancements focus on modifying biochar's physical and chemical properties, introducing novel functionalities through techniques like steam activation, thermal air treatment, acid modification, and the creation of biochar nanocomposites. Additionally, approaches such as ball milling and surface functionalization have been explored to further enhance adsorption capabilities. Recent studies have also investigated the use of magnetic biochar for efficient water remediation, demonstrating significant improvements in contaminant removal. Table 3 provides a comprehensive overview of the various innovative methods and their results in the field of biochar-based adsorbents for water remediation as discussed in this section, highlighting the versatility and efficiency of biochar in pollutant removal.

6.2. Nanomaterials in adsorption

Recent advancements in nanotechnology have revolutionized water remediation through the development of innovative nano-adsorbents. These materials are engineered to effectively remove pollutants from water, leveraging novel fabrication methods that enhance their adsorption capacity and efficiency. Through the utilization of green synthesis, magnetic nanoparticle composites, and bio-inspired approaches, researchers have created nano-adsorbents with exceptional removal efficiencies for a variety of contaminants. Such innovations not only improve the adsorption kinetics but also introduce novel surface modifications, making water remediation more sustainable and efficient. Table 4 concisely summarizes recent research findings, highlighting unique features and efficiencies of various nano-adsorbents in water remediation.

6.3. Metal organic framework based adsorbents

Recent studies have explored novel approaches in MOF-based adsorption, focusing on the synthesis and functionalization of MOFs for enhanced performance in water remediation. These advancements include the creation of aerogel composites, bio-nano-composite beads, bimetallic MOFs, and the utilization of amorphous MOFs synthesized in deep eutectic solvents. These approaches have shown significant improvements in adsorption capacities and selectivity towards various pollutants. The detailed outcomes of these innovative strategies are summarized in Table 5, highlighting the synthesis methods, main findings, and contributions of the research groups involved.

6.4. Membrane-based adsorption techniques

Membrane-based adsorption techniques have significantly advanced water remediation efforts, merging adsorptive material properties with selective membrane separation. These innovations have led to enhanced efficiency and sustainability in treating various pollutants, including heavy metals, organic compounds, and emerging contaminants. Recent case studies have introduced novel adsorptive materials and membrane configurations, showcasing a range of promising developments from increased adsorption capacities to improved selectivity and stability. Table 6 provides an overview, emphasizing the synthesis methods, performance outcomes, and the researchers behind these advancements.

Table 3
Various novel techniques and outcomes in the field of biochar-based adsorbents for water remediation.

Reference	Method/Approach	Biochar Source	Key Findings/Results
[76]	Steam activation	Invasive plant derived	Surface area increased from 2.3 to 7.1 m^2/g; adsorption of sulfamethazine improved
[77]	Thermal air treatment	Wood derived	Nine-fold increase in tetracycline adsorption capacity
[60]	Acid modification (H_3PO_4)	Rice straw derived	Increased surface area and hydrophobicity; 25 % improvement in tetracycline adsorption
[78]	NaOH modification	Bamboo derived	Tripling of adsorption capacity for chloramphenicol
[79]	Hydrothermal synthesis	Magnetic $CuZnFe_2O_4$-biochar composite	65 % higher sulfamethoxazole adsorption
[80]	Coating with TiO2 nanoparticles	Reed straw derived	91 % SMX degradation under UV irradiation
[81]	Ball milling	Peanut shell biochar	96 % removal efficiency for Cd(II)
[82]	Ball milling	Hickory wood biochar	High adsorption capacities for VOCs like acetone, cyclohexane, and toluene
[83]	Amino-functionalized silica coating	Magnetic nano-biochar	High removal capacities for Cu(II) and Pb(II)
[84]	Ethylenediamine functionalization	Nano-biochar	Effective removal of Cr(VI) and prednisolone
[85]	Mg/Zr modification	Nano-biochar from spent coffee grounds	87 % phosphate removal rate
[86]	Nanoscale preparation	Rice husk biochar	78 % fluoride removal from contaminated water
[87]	Electromagnetic induction pyrolysis	Cellulose and $FeCl_3$	95.9 mg/g Cr(VI) removal capacity
[88]	Seawater minerals for magnesium ferrite doping	Jackfruit peel and potassium ferrate	61.30 mg/g Cu^{2+} ions adsorption capacity
[89]	One-step hydrothermal method	Bamboo and $FeCl_3{\cdot}6H_2O$	Remarkable uptake of U(VI) ions
[90]	Hydrothermal synthesis	Avocado peels and $FeCl_3{\cdot}6H_2O$	Methylene blue adsorption capacity of 250 mg/g
[91]	Impregnation pyrolysis	Rice straw and stainless steel pickling waste liquor	71.91 % crystal violet removal

Table 4
Overview of some recent nano-material based adsorbents for water remediation.

Reference	Nano-material	Contaminant Removed	Adsorption Capacity	Key Features
[92]	CSL-NanoB	Cd(II), Sm(III)	Cd(II): 1150 μmol/g, Sm(III): 650 μmol/g	Crafted from Cynara scolymus leaves, uniform nanosized structure, eco-friendly
[93]	Iron oxide-silica nanocomposite	Methyl orange, Pb^{2+}	Methyl orange: 240 mg/g, Pb^{2+}: 50 mg/g	Superparamagnetic, mesoporous silica coating, large surface area
[94]	CAZ	Fluoride ions	249 μmol/m2 (216 mg/g)	Loaded calcium and zirconium oxides on alumina
[95]	MWCNTs	Diazinon	100 % removal efficiency	Multi-wall carbon nanotubes, effective for pesticide removal
[96]	Co_3O_4 nanoparticles	Methyl orange	46.08 mg/g	Hexagonal sheet-like morphology, 10–20 nm size, crystalline
[97]	$CrFeO_3$-NPs–AC	Methyl violet (MV)	65.67 mg/g	Hydrothermal synthesis, antibacterial, optimal for MV removal
[98]	PMMNs	Cr(VI)	35.186 mg/g	Polyacrylamide modified magnetic nanoparticles
[99]	ZnO-NRs-AC	Safranin O (SO)	32.06 mg/g	ZnO nanorods on activated carbon
[100]	IMGO	MV, MG dyes	MV: 172.96 mg/g, MG: 195.64 mg/g	Magnetic iron-manganese oxide coated graphene oxide
[101]	D-GSH	MV, CR dyes, Pb^{2+}, Cd^{2+}	MV: 2564 mg/g, Pb^{2+}: 781 mg/g, Cd^{2+}: 793 mg/g	Graphene sand hybrid, high capacity, environmentally friendly

Table 5
Overview of some recent advances in metal organic frameworks for water remediation.

MOF Type	Synthesis/Method	Main Findings/Performance	Reference
Nanocellulose-MOF-801 composite aerogel	Self-cross-linking	93.86 % Cr(VI) removal, 350.64 mg/g adsorption	[102]
UiO-66/CB bio-nano-composite bead	Freeze-casting and gelation	>47.9 mg/g sorption, reduces As(III) to <10 μg/L	[45]
Zr-MOF with L-tyrosine	Solvothermal method	Cu(II) removal, 79.34 mg/g adsorption	[103]
Bimetallic MOFs (Fe family elements)	One-pot flux, MOF-on-MOF	1935.68 mg/g for Congo red adsorption	[104]
Amorphous UiO-66 MOF	Deep eutectic solvent	>1300 mg/g profenofos removal	[105]
Fe-BTC-MOF composite	Solvothermal synthesis	55 mg/g Cu(II), 57 mg/g As(III), 147 mg/g Pb(II), and 155 mg/g Hg(II)	[106]
SNN-MIL-125(Ti)@Fe_3O_4 composite	Functionalization with magnetic materials	668.98 mg/g Hg ion adsorption	[107]
UiO-66-SO_3H MOF	Solvothermal method	97 % Cd and 88 % Pb removal	[108]
MPN@NH_2-MIL-101 (Fe) composite	Magnetized biomass composite	14.0 ± 0.3 mg L^{-1} phosphate adsorption	[109]
ODSOSS/TiO2/Ni-MOF/PDA@Sponge	In-situ supersaturated coprecipitation	Nearly 100 % MPs (40 mg/L) and 71.6%–95.1 % pesticides removal (10 mg/L)	[110]

Table 6
Overview of some recent advances in membrane based adsorption technologies for water remediation.

Membrane Type	Synthesis/Method	Main Findings/Performance	Reference
Multilayered Molecularly Imprinted Composite	Incorporating porous carbon nanospheres and polydopamine	2.72× surface area increase, improved hydrophilicity, 51.40 mg/g phenol adsorption, perm-selectivity >7.6	[111]
Magnetic Ion-Imprinted PAN	Polyacrylonitrile electro-spun nanofibers	130.0 mg/g adsorption for Pb(II), selectivity coefficient of 2504	[112]
MIL-53-NH_2 MOF/CA Membrane	In-situ incorporation of MIL-53-NH_2 MOF	Adsorption of chlorpyrifos increased from 160.36 to 356.34 mg/g	[113]
PVA Nanocomposite Films	Incorporation of magnetic GO-Ni-Fe_2O_4 nanoparticles	Heavy metal removal efficiency 81–98 % of 5–20 mg/L, improved mechanical/thermal properties	[114]
Poly-cyclodextrin and ZnO Nanofibrous	Electrospinning and atomic layer deposition	Surface area increase, photocatalytic activity 83.1 %–94.3 % (10–20 mg/L)	[115]
Graphene Oxide Polyamidoamine Membranes	Interfacial polymerization	Water permeability 35.89–61.52 $L/m^2\ h^{-1}$, 100 % (100 mg/L) rejection of contaminants	[71]
PAA@NM88B/GO Membrane	Vacuum filtration	98.79 % (20 mg/L) removal of methylene blue, photo-Fenton catalysis	[116]
Poly(amide-sulfonamide) Composite Membrane	Surface activation assisted multi-step polymerization	(>99.3 % of 0.1 gL^{-1}) colour removal in acidic wastewater treatment	[117]
TA-Fe Nanofiltration Membrane	Tannic acid and ferric ions coordination complexes	(>91.9 % of 10 mg/L) rejection rates of antibiotics in saline wastewater	[118]
Reactive Layer-by-Layer Assembly Membrane	Covalently-bonded polyelectrolyte layers	194 mg/g adsorption capacity for heavy metals	[46]

6.5. Machine learning and AI in adsorption optimization

The introduction of Machine Learning (ML), Artificial Intelligence (AI), and computational techniques like molecular simulations in the realm of water treatment, particularly through adsorption technologies, marks a significant advancement in environmental engineering. The fusion of these methodologies has fundamentally enhanced the precision and efficiency of identifying and optimizing adsorbents for pollutant removal [4].

The workflow in AI/ML projects encompasses problem formulation, dataset construction, model training, evaluation, and deployment. This process begins with understanding the available data, which informs model and algorithm selection. The construction of a dataset involves collecting, inspecting, processing, and visualizing data to ensure the model's reliability. Training the model involves iterative adjustments to minimize the loss function, a critical step for enhancing the model's predictive performance. Evaluation metrics play a crucial role in validating the model's accuracy and reliability across different datasets. Validation and evaluation distinguish between regression and classification models through various metrics like Mean Absolute Error (MAE) and Root Mean Square Error (RMSE), aiming for high predictive quality not just on the training set but across all data sets. The challenge of over-fitting and under-fitting is addressed through strategies that enhance the model's generalizability, such as adjustments in regularization parameters and the use of cross-validation methods [119]. Fig. 4 illustrates the workflow of application of a machine-learning model.

Molecular simulations, particularly those utilizing Density Functional Theory (DFT), have played a crucial role in predicting the capacity of adsorbents. These simulations streamline the experimental phase by evaluating the effectiveness of adsorbents against particular pollutants, thereby lessening the experimental burden. Additionally, they elucidate the mechanisms of adsorption and the interactions between pollutants and adsorbents [120]. The capabilities are further enhanced by Molecular Dynamics (MD) and Monte Carlo simulations, which offer a comprehensive insight into contaminant behaviours and the ability to predict real-time adsorption processes across a spectrum of pollutants. MD simulations, utilizing algorithms like Verlet and force fields such as CHARMM and AMBER, have been particularly effective in exploring interactions of contaminants with adsorbents. They have been applied in assessing the adsorption efficiency of materials like polyether block amide membranes, revealing insights like the impact of cavity size on adsorption capacity. Monte Carlo simulations offer a macroscopic perspective, focusing on statistical descriptions of adsorption and optimizing wastewater treatment designs, though they fall short in capturing dynamic molecular interactions [121–123]. Another critical tool, Computational Fluid Dynamics (CFD), offers insights into fluid dynamics and flow patterns within treatment systems, aiding in the design optimization of treatment units. However, CFD models, despite their utility, generally provide a more macroscopic view and might not capture atomic-level processes as effectively [121]. The role of ML in this context is significant, offering the ability to predict adsorption capacities by analysing large datasets, encompassing adsorbent characteristics and wastewater compositions. This approach significantly enhances prediction accuracy while reducing the resources required for experimental trials.

AI methods such as k-Nearest Neighbor (k-NN), Decision Trees (DT), Random Forests (RF), Artificial Neural Networks (ANNs), and Support Vector Machines (SVM) have been widely utilized in the field of water treatment. These methodologies excel in tasks such as regression, classification, and pattern recognition, significantly enhancing the performance of adsorbents for pollutant removal. ANNs, for instance, are adept at modelling complex systems with nonlinear relationships, while SVMs are effective in high-dimensional

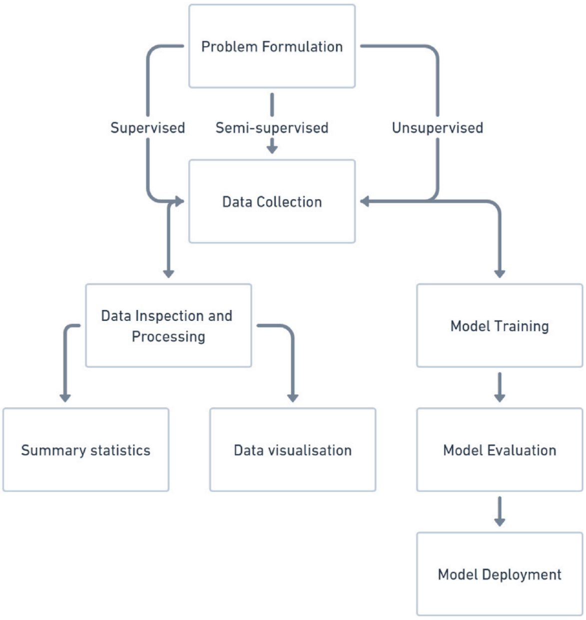

Fig. 4. Process flow of utilizing a machine-learning model.

datasets. Genetic Algorithms (GA) and Particle Swarm Optimization (PSO) are pivotal in optimizing processes, emulating natural evolutionary processes and swarm intelligence [3]. The incorporation of machine learning (ML), artificial intelligence (AI), and computational approaches is transforming water remediation, especially with the use of adsorption technology. Nevertheless, employing AI in water treatment comes with its set of challenges. Notable limitations include the requirement for extensive historical data for training AI models and the associated computational expenses. Despite these challenges, ongoing research and development are crucial for fully leveraging the immense potential of AI in transforming water treatment processes. These methods, with their unique strengths and limitations, collectively provide a comprehensive toolkit for optimizing adsorption processes. The future of AI in water treatment is promising, poised to play a pivotal role in advancing technologies and contributing to environmental protection and sustainable development. Table 7 presents a compilation of different ML and AI tools employed to improve the effectiveness of adsorption in water remediation.

7. Comparative evaluation of adsorption techniques

Adsorption methods have been extensively researched and utilized for various environmental purposes over the years. The evolution of these techniques from traditional methods to modern approaches has been marked by significant advancements in materials science and process engineering. Traditional methods, often relying on activated carbon and zeolites, have provided a strong foundation for the development of modern techniques that utilize advanced materials like carbon nanotubes and graphene-based structures [124]. The comparative evaluation of these techniques reveals a complex landscape where factors such as efficacy, efficiency, cost, and environmental impact interplay to determine the best solution for a specific application. The subsections below delve deeper into these aspects, providing a structured comparison and highlighting the latest advancements in the field.

7.1. Traditional vs. modern adsorption methods

In the context of water remediation, adsorption methods have evolved significantly from traditional to modern techniques, reflecting advancements in materials science and environmental engineering. Traditional adsorption methods primarily utilized natural adsorbents like activated carbon, clay minerals, and biochar. These materials, while effective in certain contexts, often had limitations in terms of adsorption capacity, selectivity, and regeneration ability [47,125]. Modern adsorption techniques, on the other hand, have embraced nanotechnology and advanced material synthesis. These include the use of metal oxides, carbon nanomaterials, dendritic polymers, and nanostructured adsorbents. These materials have a higher capacity to adsorb pollutants, can target specific pollutants with greater accuracy, and can be regenerated more efficiently. For instance, graphene oxide-zinc oxide nanocomposites have shown effectiveness in removing heavy metals from wastewater, and polysaccharide-based materials have been developed for the adsorption of toxic pollutants, offering low-cost solutions for environmental protection [39]. The principle of adsorption remains largely the same across traditional and modern methods, relying on the surface interaction between the adsorbent and the adsorbate. However, modern adsorbents often have engineered surfaces with specific functional groups or structures that enhance their affinity for certain pollutants. This specificity is particularly important in the context of complex wastewater streams containing a mix of contaminants. In terms of synthesis techniques, traditional adsorbents like activated carbon are typically produced through physical or chemical activation processes. Modern adsorbents, however, often require more sophisticated synthesis methods, including nanofabrication techniques, to achieve the desired structural and chemical properties. The adsorption limits of these materials vary widely, depending on their composition and structure. For example, nanostructured adsorbents can achieve much higher adsorption capacities compared to traditional materials due to their larger surface areas and tailored interaction sites [9,21]. Table 8 provides a nuanced comparison, illustrating how modern adsorption methods have advanced in terms of material complexity, specificity, and efficiency, addressing some of the limitations of traditional methods.

Table 7

Common AI and ML tools for adsorbent development, system design and process optimization.

AI/ML Tool(s)[a]	Purpose in Water Treatment
Molecular Dynamics (MD)	To analyze the interactions of contaminants with adsorbents and predict adsorption efficiency.
Monte Carlo Simulations	For statistical analysis of adsorbent efficiency under various conditions; however, less effective in dynamic processes.
Computational Fluid Dynamics (CFD)	To model fluid dynamics and flow patterns in treatment systems, aiding in design optimization.
k-Nearest Neighbor (k-NN)	Used for regression, classification, and pattern recognition in water treatment, particularly in optimizing adsorption processes.
Decision Trees (DT)	Effective for classification and regression tasks, helping in understanding complex relationships in treatment processes.
Random Forests (RF)	Employed for predictive analytics, capable of handling large datasets and improving accuracy in pollutant removal.
Artificial Neural Networks (ANNs)	Ideal for capturing complex nonlinear relationships in water treatment processes.
Support Vector Machines (SVM)	Used for classification and regression in high-dimensional datasets, both in linear and non-linear modelling.
Self-Organizing Maps (SOM)	Applied for clustering and pattern recognition, aiding in the analysis and optimization of treatment processes.
Genetic Algorithms (GA)	Mimics natural evolutionary processes for optimization, improving process efficiency in water treatment.
Particle Swarm Optimization (PSO)	Utilizes swarm intelligence for solving optimization problems, enhancing treatment process efficiency.

[a] Some of these tools are used in conjugation with AI and deep learning models.

Table 8

Comparative analysis of traditional and modern adsorption methods in water remediation.

Aspect	Traditional adsorption methods	Modern adsorption methods
Adsorbent Type	Activated Carbon, Bentonite Clay, Biochar	Graphene Oxide-ZnO Nanocomposites, Metal Oxide Adsorbents, Dendritic Polymers
Synthesis Technique	Physical/Chemical Activation (Activated Carbon), Natural Formation/Modification (Bentonite Clay), Pyrolysis of Biomass (Biochar)	Nanofabrication (Graphene Oxide-ZnO), Chemical Synthesis/Nanofabrication (Metal Oxides), Polymerization Techniques (Dendritic Polymers)
Principle	Surface Adsorption, Ion Exchange (Bentonite Clay)	Enhanced Surface Adsorption, Chemical Interaction, Molecular Recognition
Adsorption Limit	Moderate, limited by surface area and pore structure	High, enhanced by engineered surface areas, functional groups, and nanostructures
Key Advantages	Simplicity, natural availability, cost-effectiveness	Higher efficiency, specificity for contaminants, reusability, advanced control over adsorption properties
Typical Applications	General water purification, removal of common pollutants	Targeted removal of specific contaminants, complex wastewater streams, heavy metal, and organic pollutant removal
References	[126,127]	[39,128]

Table 9

Overview of the comparative efficiency, ease of synthesis, and economic considerations of different adsorbent types in water remediation.

Adsorbent Type	Specific Pollutants Targeted	Efficiency (%)	Ease of Synthesis	Regeneration Capability	Economic Aspect	Environmental Impact
Activated Carbon	Organic compounds, Chlorinated compounds, Heavy metals	High (up to 90–95 % for organic compounds)	Moderate (energy-intensive process)	Good (can be regenerated but with diminishing efficiency)	Moderate-High (due to production and regeneration costs)	Moderate (requires energy-intensive production, but low waste generation)
Zeolites	Cations (e.g., Na+, K+), Heavy metals (e.g., Pb, Cd)	Moderate-High (varies with zeolite type and pollutant)	Moderate (less energy-intensive than activated carbon)	Moderate (ion-exchange capacity can diminish over time)	Moderate (cost-effective for specific applications)	Low (natural and synthetic varieties with minimal environmental impact)
Nano-adsorbents	Trace pollutants, Heavy metals, Organic compounds	Very High (efficient even at low concentrations)	Low (complex and costly synthesis)	Varies (some can be regenerated, others are single-use)	High (due to advanced technology and materials used)	High (concerns about stability and nano-particle release into the environment)
MOFs	Heavy metals, organic compounds, emerging pollutants	High (varies with MOF type and pollutant)	Moderate-High (can be energy-intensive)	Good (with minimal efficiency loss)	Moderate (high efficiency can offset initial costs)	Moderate (requires further research on stability and impact)
Biochar	Organic pollutants, Heavy metals, Phosphates	Moderate (50–70 % for various pollutants)	High (relatively simple production from biomass)	Low (limited regeneration capability)	Low (cost-effective, especially when produced from waste biomass)	Low (sustainable and environmentally friendly, but with variable efficiency)

7.2. *Efficacy and efficiency evaluation*

Assessing the effectiveness and efficiency of various adsorbents for water remediation is a crucial research area, especially given the rising water pollution levels and the demand for sustainable treatment approaches. Adsorbent-based water remediation techniques are favoured due to their effectiveness in removing various pollutants, ease of synthesis, and potential economic benefits. Nonetheless, the effectiveness of these adsorbents can vary considerably depending on their type and the specific characteristics of the pollutants they are intended to eliminate [129]. Comparatively, other water remediation techniques such as biological treatment, chemical oxidation, and membrane filtration have their unique advantages and limitations. Biological treatments are effective for organic pollutants but are less effective against heavy metals and inorganic compounds. Chemical oxidation can degrade a diverse range of pollutants but often requires the use of harsh chemicals. Membrane filtration is highly effective for many pollutants but can be cost-prohibitive and energy-intensive. On the contrary, approaches based on adsorbents present a flexible and frequently more economically viable solution for a diverse array of pollutants [130].

Within the spectrum of adsorbents, activated carbon stands out for its notable efficacy in eliminating organic compounds, chlorinated compounds, and heavy metals from water. Its exceptional adsorption capabilities are attributed to its extensive surface area and porous structure. However, generating activated carbon can demand significant energy, and its effectiveness might decline over time, necessitating the need for regeneration or replacement [41]. Zeolites, another category of adsorbents, are effective in removing cations, such as heavy metals, from water. Their crystalline structure allows for selective ion exchange, which can be tailored for specific pollutants. The synthesis of zeolites is less energy-intensive compared to activated carbon, but their effectiveness is largely dependent on the specific type of zeolite and the pollutant in question [42]. Nano-adsorbents, especially those derived from metal oxides and carbon nanotubes, are highly promising owing to their extensive surface area and high reactivity. These materials excel in eliminating minute quantities of contaminants, encompassing both heavy metals and organic substances. However, the synthesis of nano-adsorbents can be complex and costly, and there are concerns about their stability and potential environmental impact [131]. MOFs are emerging as highly efficient adsorbents in water remediation, known for their exceptional porosity and tunable structures. MOFs are crystalline structures made up of clusters or metal ions bonded with organic ligands. These connections create structures that can be one, two, or three-dimensional in nature. The exceptional structure of MOFs imparts them with an exceptionally expansive surface area, making them advantageous for the adsorption of a diverse array of pollutants, ranging from organic contaminants and heavy metals to emerging substances like pharmaceuticals. The production of MOFs may demand a considerable amount of energy, yet their substantial adsorption capabilities frequently validate the initial energy expenditure. Additionally, numerous MOFs can be restored with minimal efficiency loss, bolstering their economic viability. Nevertheless, the long-term viability of MOFs in water-based settings and their potential environmental consequences represent aspects that warrant additional investigation [44]. Biochar, obtained through the pyrolysis of biomass, is a rising adsorbent attracting interest for its sustainability and economical nature. It is particularly effective in adsorbing organic pollutants and heavy metals. The ease of synthesis from agricultural waste makes biochar an economically attractive option, though its adsorption capacity is generally lower than that of activated carbon [12,132]. The economic aspects of these adsorbents vary widely. Activated carbon is relatively expensive to produce but offers high efficiency, while biochar represents a low-cost, albeit less efficient, alternative. The cost of nano-adsorbents, MOFs and zeolites tends to be higher due to more complex synthesis processes, but their high efficiency can offset the initial investment in certain applications. Table 9 provides a detailed perspective on each type of adsorbent, emphasizing their effectiveness and cost aspects, as well as their regeneration potential and environmental effects.

7.3. *Cost and environmental impact analysis*

The expense associated with the preparation and application of adsorbents plays a pivotal role in wastewater treatment, especially when evaluating its feasibility compared to alternative technologies in the field. The total cost of an adsorbent can be assessed using diverse approaches, such as accounting for raw material expenses, cost indices, discounted cash flow, as well as evaluating the cost per

Table 10
Cost and environmental impact of popular adsorbents.

Adsorbent Type	Economic Aspects	Environmental Impacts	Sustainability Considerations
Biosorbents	Generally low cost, varies with source material	Often environmentally benign, biodegradable	Minimizes waste, promotes resource recovery
Activated Carbon	Can be high, depending on production method	High energy consumption in production, chemical usage concerns	Requires sustainable production and disposal methods
Biochar	Variable, often low cost	Carbon sequestration, may involve high energy consumption	Utilizes waste materials, reduces greenhouse gases
Clays & Minerals	Cost varies with material and processing	Low to moderate environmental impact	Often involves natural, abundant materials
Polymers	Varies widely, often higher than natural adsorbents	Potential chemical pollution during synthesis	Needs eco-friendly synthesis and disposal strategies
Nanoparticles	Generally high cost	Potential ecological risks, energy-intensive production	Requires careful assessment of lifecycle impacts
Composites	Highly variable, dependent on components	Depends on constituent materials	Needs careful design for environmental sustainability

gram of adsorbate removed, annual capital expenditure (CAPEX), and operating expenditures (OPEX). This comprehensive approach to cost analysis is essential for evaluating the economic feasibility of adsorbents in water treatment and their potential for scale-up from pilot to industrial scales [133]. Adsorption, as a method for pollutant removal from wastewater, stands out due to its versatility, simplicity of design, potential for adsorbent reuse, low cost, and eco-friendliness. Different categories of adsorbents, including biochar, biosorbents, activated carbon, minerals and clay, nanoparticles, polymers, and composites, are employed due to their elevated adsorption capacity, demonstrating their efficacy in eliminating harmful pollutants from wastewater. These adsorbents differ in terms of accessibility, economic viability, regenerative capability, and environmental friendliness, and they can be produced from sustainable sources. Nonetheless, reducing the cost of using these adsorbents without compromising water treatment quality remains an important goal. To standardize and compare the costs of different adsorbents, a quantitative metric known as “adsorbent cost performance” ($\hat{C}$), computed in \$/mol, was developed. Modern adsorbents differ in terms of accessibility, economic viability, regenerative capability, and environmental friendliness, and they can be produced from sustainable sources. Most of these adsorbents fall within the cost performance range of 1–200 \$/mol, with those costing less than 1 \$/mol considered very cheap and those above 200 \$/mol considered very expensive. This analysis was conducted by converting reported adsorption capacity to mol/g and cost to \$/g and determining their ratio. However, comparisons between different adsorbent classes should be made on a case-by-case basis due to variations in preparation intricacies and solution chemistry [32]. In addition to cost considerations, evaluating the environmental impact of adsorbents is a vital aspect of their comprehensive assessment. The production, usage, and disposal of adsorbents have varying degrees of environmental implications. For instance, the use of waste materials as biosorbents not only provides a cost advantage but also aligns with sustainable practices like waste minimization and resource recovery. However, some adsorbents, especially those requiring chemical activation or complex synthesis processes, may pose environmental risks, including chemical pollution and high energy consumption during production. Additionally, the proper disposal of used adsorbents, particularly those saturated with harmful pollutants, is a significant concern due to the risk of secondary pollution, underscoring the importance of selecting environmentally suitable adsorbents. Table 10 below summarizes the cost, environmental impact, and sustainability of popular adsorbents, highlighting the balance between affordability and eco-friendliness in water treatment [33,37,38].

8. Future prospects

The field of adsorption techniques for wastewater remediation is poised for significant evolution, driven by relentless research and technological innovation. The transition from conventional to advanced methods has been underpinned by groundbreaking developments in material science and environmental engineering. Traditional approaches, primarily centred around activated carbon and zeolites, have set the stage for the emergence of sophisticated techniques employing novel materials like carbon nanotubes, MOFs, and graphene-based structures. This evolution reflects a dynamic interplay of factors such as efficacy, cost-effectiveness, environmental sustainability, and technological feasibility. The following sub-section surveys the future landscape of adsorption methods in wastewater remediation, highlighting the most recent advances and promising trends in this field.

8.1. Predicted trends in wastewater remediation

In the dynamic and evolving field of wastewater remediation, a diverse array of methods has been developed, each uniquely designed to address different types of pollutants. These methods range from physical to chemical, biological and physico-chemical techniques, each with its specific mechanisms and applications. Starting with physical methods, these include techniques like

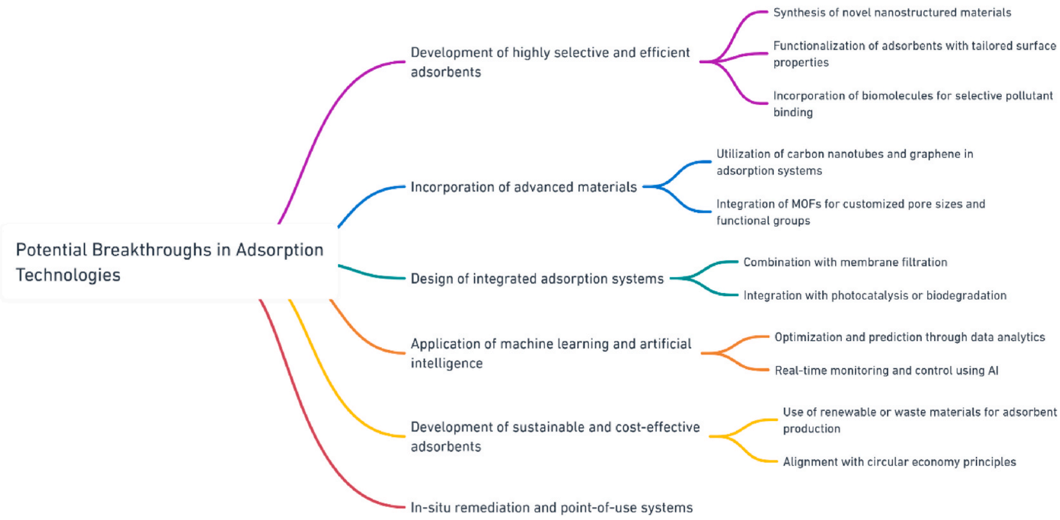

Fig. 5. Some promising directions for innovation that could transform adsorption technology.

filtration, sedimentation, and flotation. They primarily rely on the physical properties of pollutants to separate them from wastewater. These methods are straightforward and effective for certain types of contaminants [130]. Moving to chemical methods, these are distinguished by their use of various agents such as coagulants, flocculants, oxidants, and reductants. These agents work by altering the chemical characteristics of pollutants, thereby facilitating their removal. In this category, Advanced Oxidation Processes (AOPs) stand out for their ability to create reactive oxygen species, like hydroxyl radicals, which are extremely efficient in breaking down resilient organic pollutants and neutralizing pathogenic microorganisms. These processes, which include Fenton, photo-Fenton, ozonation, photocatalysis, and electrochemical oxidation, can be both homogeneous and heterogeneous in nature [134–136]. In the realm of biological methods, enzymatic treatment is a notable innovation. It employs enzymes as biocatalysts to specifically target and break down pollutants. The effectiveness of these enzymes is often enhanced when they are immobilized on various substrates, such as membranes, beads, or nanomaterials [137]. Specific enzymes such as laccase, peroxidase, nitrilase, and lipase have gained particular importance in wastewater remediation due to their ability to effectively break down and degrade complex pollutants [138]. Alongside enzymatic treatment, bioremediation techniques are also being refined. These techniques use microorganisms or plants for pollutant removal and are optimized for both in situ and ex situ applications, with methods like bioaugmentation, biostimulation, and phytoremediation showing considerable promise [139,140].

Among these diverse methods, adsorption, a physico-chemical technique, stands out for its versatility and efficiency. Adsorption works by accumulating pollutants onto the surface of adsorbents that have a high affinity and selectivity for binding specific contaminants. The effectiveness of adsorption is attributed to its broad range of adsorbents, including activated carbon, zeolites, clay minerals, biochar, metal-organic frameworks, and graphene-based materials. This method is not only cost-effective and easy to operate but also versatile in removing a wide array of pollutants like heavy metals, dyes, oils, and micropollutants. Particularly, in the context of emerging pollutants, like personal care products, pharmaceuticals, and endocrine-disrupting pollutants, adsorption technology demonstrates significant promise. These emerging pollutants, often present in trace amounts yet having considerable ecological and human health impacts, require highly selective and efficient removal methods. Adsorption provides a viable solution with its ability to efficiently capture and concentrate these contaminants, even at very low concentrations. Furthermore, adsorption can be integrated with other techniques, such as biodegradation and advanced oxidation, to create hybrid systems [47,125,141].

Adsorption efficiency is determined by the adsorbent, contaminant, and wastewater matrix parameters. Optimizing these parameters is crucial for effective treatment. This is where data-driven techniques such as machine learning (ML) and artificial intelligence (AI) come into play. They are instrumental in uncovering hidden patterns and relationships within large, multi-dimensional data sets from adsorption systems. Machine learning algorithms may be trained to understand the influence of different operational parameters on removal efficiency and anticipate results under certain situations. They also offer insights into interaction mechanisms and assist in optimizing adsorbent preparation. Additionally, ML and AI are valuable in process monitoring, control, and diagnostics, enhancing the overall efficiency and reliability of adsorption systems. Moreover, AI techniques like artificial neural networks are capable of simulating complex adsorption phenomena at the molecular level, providing insights into surface interactions and pore diffusion dynamics. These insights are invaluable for guiding the synthesis and application of adsorbents [142]. The integration of nanotechnology, advanced materials, and AI-based tools heralds a promising future for adsorptive wastewater treatment. This makes it possible to develop sustainable and intelligent technologies for the removal of both traditional and emerging contaminants. However, issues including computing requirements, data gathering, and model interpretability must be addressed. Overcoming these challenges requires collaborative efforts from material scientists, engineers, and data scientists. The potential benefits in terms of clean water and environmental health are immense and invaluable.

8.2. Potential breakthroughs in adsorption technologies

The future of adsorption technology holds exciting possibilities for further breakthroughs in water purification and environmental sustainability. Some potential areas of advancement that could revolutionize adsorption technology are illustrated in (Fig. 5) and are explained in brief in following sub-sections.

8.2.1. Development of highly selective and efficient adsorbents

Researchers are continuously exploring new materials and modifying existing adsorbents to enhance their selectivity and adsorption capacity for specific pollutants. This includes the synthesis of novel nanostructured materials, which offer a high surface-to-volume ratio, increasing the contact area for pollutant capture. Functionalizing adsorbents with tailored surface properties, such as introducing specific functional groups, can provide specific binding sites for target pollutants. Additionally, incorporating biomolecules for selective pollutant binding involves leveraging molecular recognition principles, where biological entities like enzymes or antibodies are used to capture pollutants selectively [22].

8.2.2. Incorporation of advanced materials

The development of adsorption systems that utilize advanced materials like carbon nanotubes, graphene, MOFs, and COFs has the potential to unlock significant enhancements in overall performance. Integrating carbon nanotubes and graphene, with their superior electrical, thermal, and mechanical properties, into adsorption systems can significantly improve adsorption efficiency and selectivity. MOFs' highly ordered and tunable porous nature presents a remarkable opportunity to create adsorbents with customized pore sizes and functional groups. This capability empowers MOFs to capture a diverse range of pollutants selectively [14,15,64]. Recently, COFs have received significant attention as a promising candidate in water remediation applications due to their unique structural properties. COFs are highly stable in water, have a large surface area, contain many functional sites, and have adjustable pore sizes. They are perfect for removing various water pollutants, including organic and inorganic contaminants. Moreover, exploring dynamic covalent chemistry (DCC) principles and keto–enol tautomerism, for COF synthesis in water represents a pivotal advancement in developing environmentally friendly and chemically robust frameworks for water remediation. This approach underscores the significance of water as not just a solvent but a crucial component in the green synthesis of COFs, enabling their deployment in real-world water remediation applications [143,144].

8.2.3. Design of integrated adsorption systems

Combining adsorption with other water treatment processes, such as membrane filtration, photocatalysis, or biodegradation, could create synergistic effects and expand the range of pollutants that can be effectively removed. For example, integrating membrane filtration can help in removing larger contaminants, while adsorption targets dissolved pollutants. Photocatalysis can degrade organic pollutants, complementing the adsorption process. Integrated systems could also address challenges like adsorbent regeneration and minimize waste generation, making the water treatment process more sustainable and efficient [70].

8.2.4. Application of machine learning and artificial intelligence

The use of data analytics and machine learning algorithms could optimize adsorption processes, predict pollutant removal efficiency, and develop intelligent adsorption systems that adapt to changing water conditions and pollutant compositions. Machine learning techniques can analyze intricate datasets to uncover trends in adsorption efficiency, enabling proactive maintenance and performance optimization. Artificial intelligence could also assist in the real-time monitoring and control of adsorption systems, ensuring maximum efficiency and adaptability to fluctuating water quality conditions [142]. A thorough discussion of using ML and AI in adsorption optimization is presented in (**Section 6.5**).

8.2.5. Development of sustainable and cost-effective adsorbents

Developing adsorbents from renewable or waste materials, such as agricultural residues, biomass, and industrial byproducts could reduce the environmental footprint of adsorption technology and make it more cost-effective for large-scale wastewater treatment applications. Harnessing these waste materials not only prevents them from ending up in landfills but also transforms them into valuable resources. This approach aligns with the principles of circular economy, promoting sustainability and resource efficiency [2,32].

8.2.6. In-situ remediation and point-of-use systems

Scientists are investigating the potential of adsorption technology to clean up contaminated sites directly (in situ) and to create point-of-use water treatment systems for resource-poor communities. In-situ remediation involves treating pollutants directly at the contamination source, minimizing environmental disturbance and transportation costs. Point-of-application systems, on the other hand, offer localized treatment solutions, especially crucial in areas lacking centralized water treatment facilities, thereby improving access to clean water [145].

8.2.7. Tailoring adsorbents for emerging pollutants

The development of adsorbents specifically designed to remove emerging pollutants, such as pharmaceuticals, personal care products and, microplastics is an important area of research. These emerging pollutants, often not adequately addressed by traditional water treatment methods, pose unique challenges due to their diverse chemical structures and behaviours. Tailoring adsorbents to target these specific pollutants is essential for protecting environmental and human health [47].

8.2.8. Regeneration and reuse of adsorbents

Increasing the ability to regenerate and reuse adsorbents is essential for reducing waste production and enhancing the cost-effectiveness of adsorption technology. This includes developing regeneration techniques that are energy-efficient and environmentally friendly. Effective regeneration methods can significantly reduce the operational costs of adsorption processes and minimize the environmental impact by reducing the need for new adsorbent materials [26].

8.2.9. Understanding adsorption mechanisms at the molecular level

A profound understanding of adsorption mechanisms at the molecular level holds the key to creating adsorbents with precisely controlled properties and breakthrough performance. This involves studying the interactions between pollutants and adsorbent surfaces at the atomic scale, which can reveal insights into factors influencing adsorption efficiency, such as surface chemistry, pore size distribution, and material morphology [146].

8.2.10. Integration of adsorption technology with circular economy principles

Incorporating adsorption technology into circular economy principles could foster the retrieval and repurposing of valuable resources from wastewater, thereby mitigating the environmental footprint of water treatment processes. This approach not only focuses on the effective remediation of pollutants but also emphasizes the recovery of useful substances, such as nutrients or metals, from the adsorption process, thereby turning waste into a resource and contributing to a more sustainable and circular approach to water treatment [147].

8.3. Implications for sustainability and environmental health

The application of advanced adsorption technologies for water remediation, when designed in alignment with green chemistry principles, offers significant promise for improving sustainability and environmental health. The development of novel "green" adsorbents utilizing waste materials or sustainably sourced raw materials can minimize ecological impacts and the carbon footprint associated with synthesis and lifecycle management. For example, biochar derived from agricultural, or forestry wastes have shown effectiveness for adsorptive removal of water pollutants while also providing circular economy benefits. Widespread deployment of optimized adsorption technologies powered by renewable energy sources has potential to provide cleaner water for human use and protect aquatic ecosystems on a global scale [148]. However, the toxicity of nanoscale adsorbents warrants careful assessment to ensure environmental risks do not outweigh benefits. Standardized lifecycle assessment frameworks accounting for toxicity impacts are needed to guide the design and application of nano-adsorbents. Studies suggest that green synthesis routes utilizing plant extracts can produce nano-adsorbents with lower cytotoxicity and environmental risk. Further research and development are still required to realize the full potential of green engineered adsorbents that can effectively and sustainably remediate contaminated water [148,149]. With responsible implementation and management, adsorption techniques aligned with sustainability principles represent a promising approach to securing cleaner water resources for current and future generations.

9. Conclusion

Nanotechnology and materials science advancements have significantly improved adsorption's efficiency, selectivity, and stability, showcasing its potential for advanced water purification methods. However, transitioning from laboratory breakthroughs to scalable, cost-effective, real-world applications faces obstacles, notably in adapting these innovations to practical deployment. AI and ML offer a promising solution, optimizing adsorption processes and material performance in diverse environmental settings, potentially bridging the gap between research and application. Future research must prioritize sustainable (green synthesis) and economically viable adsorption technologies, leveraging AI and ML to refine process efficiency and predictability. Collaborative efforts across disciplines are essential to translate these scientific advancements into operational solutions that are both scalable and environmentally sustainable. Developing standardized evaluation frameworks for new adsorbents' environmental and economic impacts is crucial, enabling a comprehensive understanding of their lifecycle and sustainability. By focusing on these areas, integrating innovative materials and data-driven optimization techniques can make effective wastewater treatment accessible and sustainable, aligning with global clean water access goals.

Data availability statement

Data from our study remains undeposited in any public repository as all pertinent facts and figures utilized herein are comprehensively included with appropriate references.

CRediT authorship contribution statement

Satyam Satyam: Writing – review & editing, Writing – original draft, Data curation, Conceptualization. **Sanjukta Patra:** Writing – review & editing, Supervision, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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