

## Green Innovations in Water and Wastewater Treatment: Mechanistic Insights and AI Integration

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### Abstract

The pursuit of sustainable water purification technologies has catalyzed the emergence of green materials as high-performance alternatives to conventional synthetic agents. Sourced renewably and characterized by their biodegradability and low environmental toxicity, these advanced materials represent a paradigm shift in water treatment. This review highlights the exceptional potential of natural nanomaterials—including cellulose nanofibers, chitosan, alginate, and lignin—as well as their engineered composites, functionalized hydrogels, and aerogels for the highly efficient adsorption of heavy metals, dyes, and persistent organic contaminants. A critical analysis of contaminant removal mechanisms is presented, alongside the application of advanced modeling and optimization techniques. These computational tools are indispensable for predicting material properties, simulating molecular interactions, and tailoring bespoke solutions, thereby accelerating rational design. While challenges in scalability, synthesis cost, and real-world validation remain, this work concludes that the integration of green materials with cutting-edge computational models is pivotal for developing the next generation of efficient, sustainable, and environmentally benign water treatment systems, directly supporting global sustainable development and climate action goals.

**Keywords:** Green materials; Sustainable water treatment; Natural polymers; Adsorption mechanisms; Computational modeling; Contaminant removal.

### 1. Introduction

The growing global population has made water and wastewater treatment essential to mitigate the severe pollution of water reservoirs and address the critical scarcity of drinking water [1]. This challenge is central to the 2030 Agenda on Sustainable Development, specifically Goal 6, which aims to "ensure availability and sustainable management of water and sanitation for all" [2]. This goal underscores the necessity for water to be both accessible and free of impurities, recognizing it as an indispensable natural resource for life.

To achieve this, various technological treatments are employed to ensure water quality is adequate for both consumption and safe discharge into the environment [3]. These treatments consist of a set of physical, chemical, or biological unit operations designed to eliminate or reduce contamination and undesirable characteristics [4]. The specific design of these systems depends on the contaminants present, which can include suspended solids, heavy metals, oils, fats, recalcitrant organic compounds, and emerging contaminants like antibiotics, hormones, and microplastics [5].

A critical component of these treatment systems are the materials used, which can be organic or inorganic. These materials provide efficient solutions for removing contaminants, disinfecting water, and enabling reuse [4,6]. However, a significant challenge arises from the waste generated by these processes—the concentrated contaminants removed from the water [13]. A promising solution is to apply circular economy principles to valorize this waste [14,15] or to utilize materials with inherent recyclability or biodegradability, known as **green materials**, which can be incorporated into the environment without generating pollution [7,16].

## 1.1 The Promise and Challenge of Green Materials

In the face of escalating environmental challenges, green materials have emerged as pivotal in mitigating the ecological footprint of industrial and consumer activities [20]. Characterized by their renewable origins and minimized environmental impact throughout their lifecycle, they represent a paradigm shift in sustainable practices.

Currently, one of the most widely used green materials in water treatment is activated carbon derived from lignocellulosic biomass [17,18]. However, many other green materials are still under research and have not yet achieved the performance and durability required to compete with conventional materials, especially in industrial applications that demand resilience under extreme conditions and consistent long-term performance [19]. This gap underscores the need for continuous research and development.

Green materials are primarily defined by their renewable origins, which significantly reduce dependency on fossil resources. For instance, bioplastics like polylactic acid (PLA) and starch-based polymers can emit up to 75% fewer greenhouse gases during production compared to conventional plastics [22,23]. Nevertheless, these benefits are accompanied by trade-offs, including high water and energy demands during production—a concern in water-stressed regions—and potential competition with food security when agricultural crops are used as feedstocks. This has prompted the exploration of alternative sources, such as lignocellulosic biomass or agro-industrial residues.

Despite these limitations, demand for green materials continues to grow, driven by a cultural and economic shift towards sustainability. Both consumers and industries are increasingly prioritizing solutions that reduce environmental impact and contribute to climate change mitigation. This shift in market preferences is encouraging manufacturers to invest in innovation to develop materials that are more affordable, high-performing, and environmentally friendly [22].

## 1.2 Aim and Objectives of This Research

Therefore, the aim of this research is to review the current status of green materials applied in water and wastewater treatment, as they are presented as a key tool to address global challenges associated with climate change and the depletion of natural resources.

**Specifically, our objectives are to:**

1. Present the basic concepts and most common classifications of green materials.
2. Detail their mechanisms of action within water and wastewater treatment systems.
3. Integrate the role of natural-origin nanomaterials or those produced by green synthesis, as they represent innovative solutions with a high capacity for adsorbing emerging pollutants and heavy metals at the nanometric scale.
4. Explore the use of modeling and optimization techniques for the design and application of these materials, as these tools are vital for predicting properties, simulating interactions, and customizing solutions based on specific water characteristics.

Overall, the diversity and unique properties of green materials, combined with advanced modeling and optimization techniques, are essential to boosting sustainability and efficiency in water management, addressing both current and future challenges.

## 2. Literature Review

The global challenge of water scarcity and pollution, exacerbated by a growing population, has made advanced water and wastewater treatment essential for achieving Sustainable Development Goal 6, which aims to ensure water availability and sustainable management for all [1, 2]. Conventional treatment systems rely on a suite of physical, chemical, and biological operations to remove a complex array of contaminants, from suspended solids and heavy metals to emerging threats like microplastics and pharmaceuticals [3, 4, 5]. While effective, these processes often depend on materials derived from non-renewable resources and can generate secondary waste streams, highlighting a critical need for more sustainable solutions [12]. This has catalyzed a paradigm shift towards a circular economy model within the water sector, focusing on waste valorization and the development of **green**

**materials**—characterized by their renewable origins, minimized environmental footprint, and biodegradability—as a key tool for sustainable water management [7, 13, 14, 15, 16, 17].

The most established green material is activated carbon derived from lignocellulosic biomass, prized for its high surface area and effectiveness in adsorbing organic pollutants [18, 19]. However, the field has expanded significantly to include a diverse range of materials. Biopolymers like chitosan, cellulose, alginate, and starch are being extensively researched for their abundance, functionality, and ability to be engineered into adsorbents, flocculants, and membrane composites for removing heavy metals and dyes [33, 34, 35, 39, 40]. A particularly innovative advancement is the green synthesis of nanomaterials, where plant extracts are used to produce nanoparticles of iron, copper, silver, or zinc oxide, offering a sustainable route for creating highly reactive agents used in catalysis, disinfection, and adsorption [26, 27, 44, 48]. These materials can be further enhanced into hybrid composites, such as biopolymer-magnetic particle systems, which combine high adsorption capacity with easy magnetic separation from treated water [50, 51].

The functionality of these green materials is governed by multiple mechanisms, including adsorption onto their surfaces, ion exchange, photocatalytic degradation of organics, and even serving as a substrate for beneficial microorganisms [55, 56, 58, 59]. To optimize these complex processes and tailor materials for specific contaminants, the field is increasingly turning to computational modeling and artificial intelligence. Tools like Artificial Neural Networks (ANN) and Adaptive Neuro-Fuzzy Inference Systems (ANFIS) are now crucial for predicting synthesis outcomes, modeling adsorption kinetics, and determining optimal operational parameters, thereby reducing experimental burdens and enhancing efficiency [28, 29, 60, 62].

Despite their immense promise, green materials face significant challenges before achieving widespread industrial adoption. Key hurdles include scaling up production from the laboratory while maintaining cost-effectiveness, ensuring long-term durability and performance under real-world conditions to compete with conventional materials, and conducting comprehensive life cycle assessments to verify their overall environmental benefits [20, 65, 66]. Nevertheless, driven by a cultural and economic shift towards sustainability, ongoing research into advanced functionalization, compositing, and integration with circular economy principles continues to advance these materials [21, 23]. The synergy between the unique properties of diverse green materials and the predictive power of modern optimization techniques positions them as indispensable components for developing the efficient and sustainable water treatment technologies required to meet future global challenges [30, 31].

### 3. Definition and Criteria of Green Materials

Green materials are defined as those specifically engineered to minimize environmental impact throughout their entire life cycle, from production to disposal. Often derived from renewable sources like plants or recycled content, these materials are developed with the core purposes of conserving resources, reducing waste generation, and minimizing pollution [23]. A primary characteristic is their renewable origin, which significantly reduces dependence on finite, non-renewable resources such as fossil fuels [24]. The production processes for these materials are designed with sustainability principles at the forefront, prioritizing efficiency to decrease energy consumption, water usage, and greenhouse gas emissions [26]. For instance, bioplastics like polylactic acid (PLA) and starch-based polymers can emit up to 75% fewer greenhouse gases during their manufacturing compared to conventional plastics [25, 26].

Furthermore, green materials are typically non-toxic or of low toxicity, ensuring safety for both human health and the environment, which promotes their acceptance across a wide range of applications [27]. They also play a crucial role in enhancing energy efficiency in sectors like construction and manufacturing, thereby reducing long-term operational costs and mitigating associated carbon footprints [28]. A critically relevant aspect is their end-of-life management; many are designed for recycling or biodegradation, facilitating their integration into circular economy models. This helps manage resources sustainably and can significantly reduce waste generation [29]. For example, poly(butylene succinate) (PBS) can achieve complete degradation within six months under industrial composting conditions. However, its breakdown is markedly slower in natural environments due to suboptimal microbial activity and conditions [20]. This discrepancy underscores the vital importance of developing appropriate waste management infrastructure to realize the full biodegradability potential of such materials. Without robust end-of-life

systems, even biodegradable materials risk contributing to landfill accumulation, ultimately undermining their core sustainability objectives.

The versatility of green materials is reflected in their applications across various sectors. In construction, the use of sustainable materials like bamboo, recycled wood, and low-VOC (volatile organic compound) paints has proven effective for reducing the environmental footprint of building projects [30]. In packaging, biodegradable plant-based polymers and recycled paper offer a sustainable alternative to conventional plastics. The textile industry employs eco-friendly fabrics such as organic cotton and recycled polyester to decrease its environmental impact by reducing chemical and water consumption [20]. The electronics sector is developing devices that use recycled materials and feature recyclable designs to minimize e-waste [31], while transportation incorporates biofuels and recyclable materials to improve efficiency and reduce emissions [32].

In the specific context of water and wastewater treatment, the development and application of advanced green materials are guided by fundamental criteria such as biodegradability, low toxicity, the utilization of renewable resources, and a positive life cycle assessment. These criteria are essential for ensuring the long-term sustainability of treatment processes, protecting public health, and minimizing the environmental impact of purification technologies [33]. Conventional materials like activated carbon, alum, and chlorine, while effective for decades in removing traditional contaminants such as organic matter, heavy metals, and microorganisms [34, 35], carry significant environmental drawbacks. These include greenhouse gas emissions and the generation of hazardous waste [36]. Their effectiveness can also be limited against emerging contaminants or trace levels of certain compounds [37].

In contrast, green materials offer a more sustainable approach. Frequently derived from renewable sources like agricultural waste or natural minerals, they are associated with production processes that have a lower environmental footprint [38]. A distinct advantage is their ability to be specifically designed or functionalized to target particular contaminants, making them highly versatile. Furthermore, their biodegradable nature significantly reduces the risk of long-term environmental damage [39]. For example, cellulose nanofibers derived from lignocellulosic biomass can exhibit specific surface areas exceeding 300 m<sup>2</sup>/g, making them highly effective adsorbents for heavy metals and organic pollutants [40,41]. When integrated into polymeric membranes, these nanomaterials can enhance filtration efficiency and mechanical stability, achieving contaminant removal rates of up to 95% in wastewater treatment systems [41].

A particularly effective category is composite materials, which combine renewable components with synthetic matrices to enhance properties like mechanical strength, thermal stability, and adsorption capacity. For instance, biopolymer-clay composites merge the high adsorption capacity of clays like montmorillonite with the functional versatility of biopolymers such as chitosan, enabling the effective removal of heavy metals and dyes under diverse environmental conditions [42]. Similarly, the incorporation of zinc oxide nanoparticles into biopolymer matrices has been shown to significantly improve the photocatalytic degradation of organic pollutants, achieving reduction efficiencies exceeding 80% under UV irradiation [43]. While a conventional classification system provides a foundational framework, the true diversity and multifunctionality of advanced green materials are better captured by expanding the framework to include additional criteria such as origin (bio-based, recycled, natural), key properties (energy efficiency, environmental impact, durability), and primary applications. This nuanced understanding highlights how bio-based materials like cellulose and chitosan offer renewable alternatives for filtration and adsorption, while recycled materials contribute to resource circularity by repurposing industrial or consumer waste.

#### 4. Classification of Advanced Green Materials

Advanced green materials are essential for addressing urgent environmental challenges, particularly in water treatment and contaminant remediation. A precise understanding of their classification allows for a more accurate characterization of their properties and applications, thereby maximizing their potential for specific uses. Following a categorization system such as that proposed by Kumar [31], advanced green materials can be broadly classified into two main categories: green nanomaterials and composite materials.

#### 4.1. Green Nanomaterials

Green nanomaterials are derived from renewable natural resources such as cellulose, chitosan, lignin, alginate, and pectin. Their nanoscale design endows them with unique and enhanced properties, including a high surface area-to-volume ratio, intrinsic biodegradability, and versatile surfaces amenable to chemical functionalization [38]. These properties collectively make them highly effective for applications in advanced water treatment and targeted contaminant removal. Their small size and reactive surfaces allow for efficient adsorption, catalytic degradation, and filtration of pollutants at scales unachievable by their bulk counterparts.

**Table 1: Comparison of Green Nanomaterials from Renewable Resources**

Material	Origin	Chemical Structure Highlights	Primary Applications in Water Treatment	Key References
<b>Cellulose Nanofibers (CNF)</b>	Plant biomass (e.g., wood, agricultural residues)	Linear chain of $\beta(1 \rightarrow 4)$ linked D-glucose units; abundant hydroxyl groups for modification.	Adsorption of heavy metals and organic dyes; reinforcement in filtration membranes.	[40, 41]
<b>Chitosan Nanomaterials</b>	Crustacean shells (e.g., shrimp, crab)	Linear polysaccharide of $\beta(1 \rightarrow 4)$ linked D-glucosamine and N-acetyl-D-glucosamine; free amino groups for cation binding.	Chelation and removal of heavy metal ions; flocculation of suspended solids.	[35, 36]
<b>Lignin Nanoparticles</b>	Woody plants, pulp & paper industry waste	Complex, cross-linked phenolic polymer.	Adsorption of organic contaminants; platform for drug delivery in remediation.	[44]
<b>Alginate-Based Nanomaterials</b>	Brown seaweed (Phaeophyceae)	Linear copolymer of $\beta$ -D-mannuronate and $\alpha$ -L-guluronate.	Encapsulation of reactive agents (e.g., nano-zero-valent iron); formation of hydrogel beads for dye removal.	[42, 43]
<b>Pectin Nanoparticles</b>	Fruit peels (e.g., citrus, apple)	Heteropolysaccharide rich in $\alpha(1 \rightarrow 4)$ linked D-galacturonic acid.		

#### 4.2. Composite Materials

Composite materials represent a sophisticated class of advanced green materials engineered to overcome the inherent limitations of individual components by synergistically combining their properties. This approach results in structures with enhanced characteristics, such as superior mechanical strength, improved thermal stability, and optimized adsorption capacities, making them highly effective for complex environmental applications.

A prominent strategy involves combining biopolymers with inorganic substrates. For instance, integrating biopolymers like chitosan with clays such as montmorillonite leverages the high surface area and cation exchange capacity of the clay with the abundant functional groups (e.g., amino groups in chitosan) of the biopolymer. This synergy creates a composite capable of efficient adsorption of heavy metals and dyes, even under challenging environmental conditions [42]. Another approach combines the best of both natural and synthetic polymers. Hydrogels formulated from biopolymers (e.g., alginate) and synthetic polymers (e.g., polyacrylamide) merge the biodegradability and sustainability of the former with the mechanical robustness and durability of the latter. This makes them particularly suited for demanding, large-scale industrial applications where mechanical integrity is crucial [49]. Furthermore, the incorporation of functional nanoparticles into biopolymer matrices significantly enhances their capabilities. Embedding zinc oxide (ZnO) nanoparticles, for example, introduces powerful photocatalytic and antimicrobial properties. Studies have demonstrated that such composites can achieve reduction rates exceeding 80% in the degradation of organic contaminants under UV irradiation, while also effectively disinfecting water, thereby broadening their utility in potable water treatment systems [43, 50].

**Table 2: Components, Key Properties and Applications of Composite Green Materials**

Composite Material	Components	Key Properties	Main Applications	References
<b>Biopolymer-Clay Composites</b>	Chitosan, Montmorillonite	High adsorption capacity, Thermal stability	Heavy metal and dye remediation	[42]
<b>Biopolymer-Synthetic Polymer Composites</b>	Alginate, Polyacrylamide	Mechanical strength, Durability, Biodegradability	Industrial-scale water treatment	[49]
<b>Metal Nanoparticle-Biopolymer Composites</b>	Zinc Oxide, Biopolymers	Photocatalytic, Antimicrobial	Organic pollutant degradation, Disinfection	[43, 50]

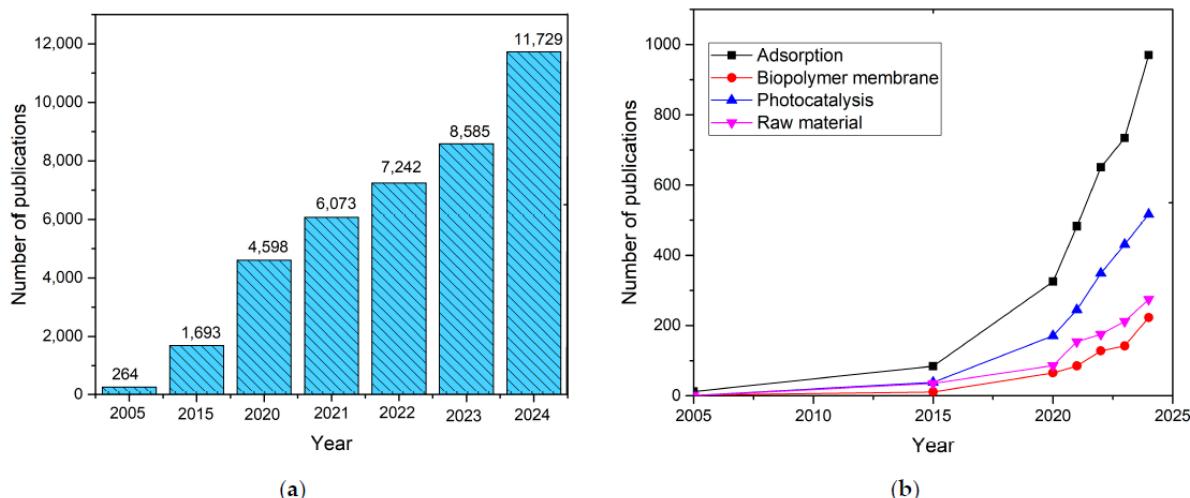
In this regard, composite materials offer a powerful and versatile alternative in the design of advanced solutions for water treatment. Their development hinges on the strategic integration of biopolymers with other components, such as clays, synthetic polymers, and photocatalysts [49]. The resulting synergy profoundly improves key functionalities like adsorption kinetics, degradation efficiency, and filtration performance, tailoring them for specific applications. A clear example is the incorporation of zinc oxide nanoparticles into polymeric matrices, which has shown a notable improvement in the photocatalytic degradation of organic contaminants under UV irradiation, highlighting its significant potential for advanced water treatment technologies [43]. Similarly, combining biopolymers with inorganic materials like montmorillonite has proven effective in enhancing the thermal and mechanical stability of the resulting composites, thereby expanding their applicability in adverse environmental conditions [51]. Furthermore, the functionalization of biopolymers with specific chemical groups enables the development of composites with greater selectivity and affinity for target pollutants, such as heavy metals, offering highly efficient and tailored solutions for water remediation [52]. These advancements firmly position composite materials as a cornerstone innovation in the development of next-generation water treatment technologies, distinguished by their high efficiency, adaptability, and ability to meet contemporary environmental challenges.

## 5. Applications of Advanced Green Materials in Water and Wastewater Treatment

Advanced green materials—derived from renewable natural resources and prepared through green synthesis or composite formation—offer significant potential for revolutionizing sustainable water and wastewater treatment. These materials possess unique properties, such as high reactivity, biodegradability, and tunable functionality, which make them highly attractive as alternatives to conventional treatment methods [38, 43]. The growing scientific and technological interest in this field is quantitatively underscored by a keyword search performed on the ScienceDirect database. Using "green material" alongside key process terms, **39,920 articles** were identified to date, highlighting the substantial and rapidly expanding research dedicated to this critical area [53].

Analysis of publication trends over the past two decades reveals a remarkable acceleration in research activity. **Figure 1a** illustrates this pronounced increase in the number of scientific articles published annually, reflecting a growing global commitment to developing sustainable solutions for water pollution challenges [54].

Furthermore, **Figure 1b** delineates the trend in research focus based on the primary processes and applications of these green materials within water and wastewater treatment systems. The data indicates that the vast majority of scientific articles concentrate on harnessing **adsorption mechanisms** and **photocatalysis** for contaminant removal, leveraging the high surface area and catalytic properties of nanomaterials like cellulose nanofibers and green-synthesized metal oxides [40, 43, 50]. This is followed by a significant research effort dedicated to the development and application of materials derived from **renewable raw materials**, such as agricultural waste, and the engineering of **biopolymer membranes** for advanced, sustainable filtration applications [41, 49]. This distribution highlights the primary pathways through which green composites are making an impact: directly sequestering pollutants, catalytically degrading them, and physically separating them through eco-friendly membranes.



A comprehensive understanding of the mechanisms that drive the remediation process using green materials is vital for identifying the key parameters that influence their effectiveness. This knowledge enables the selection and optimization of materials, thereby improving their success in pollutant degradation and removal applications. As illustrated in **Table 3**, a diverse array of advanced green materials—including aerogels, nanoparticles, membranes, and biofilms fabricated from sustainable feedstocks like agricultural waste and expired oils—demonstrate outstanding remediation efficiencies through mechanisms such as adsorption, photocatalysis, and ultra-filtration. Notable examples include the removal of Cr(VI) at 97%, Cd<sup>2+</sup> at 98.46%, Pb<sup>2+</sup> at 97.14%, acetaminophen at 75.4–84.6%, and various dyes at rates exceeding 90% [53-70]. Hybrid materials, such as chitosan/polyaniline nanofibrous composites and functionalized membranes, are particularly noteworthy for their ability to combine advanced functional properties with inherent sustainability. However, significant research challenges remain, particularly concerning material regeneration, long-term economic viability, and a thorough assessment of the potential environmental impact of leached nanoparticles. To maximize their real-world impact, future efforts must focus on industrial scale-up, enhancing material stability in complex environments, and developing hybrid applications that align with circular economy principles [53, 71].

**Table 3: Advanced Green Materials in Water and Wastewater Treatment**

Green Materials	Pollutant/% Removal/Qmax (mg/g)	Mechanism	Raw Material/Form	Reference
Biochar (BC)/reduced	Cr(VI) / 15.6 mg/g	Adsorption	Agricultural waste	[53]

Green Materials	Pollutant/% Removal/Qmax (mg/g)	Mechanism	Raw Material/Form	Reference
graphene oxide (rGO) aerogel				
Magnetite and zeolite (ZSM)/Fe <sub>3</sub> O <sub>4</sub>	Acetaminophen / 75.4–84.6%	Photocatalysis	Metal nanoparticles	[54]
Cuttlefish bone (CFB)	Malachite green / 92%	Photocatalysis	Particles	[55]
Tamarindus indica magnetic biochar (nM-BC)	Malachite green / 5.577 mg/g; Methylene blue / 3.055 mg/g	Adsorption	Seed biochar	[56]
Soybean oil bio-based material	CHCl <sub>3</sub> - dyes	Adsorption	Expired oil	[57]
NiFe <sub>2</sub> O <sub>4</sub> /Starch-g-poly(acrylic acid-co-acrylamide) (SANCH)	Cr(VI) / 99.7%	Adsorption/Photocatalysis	Hydrogel	[58]
TiO <sub>2</sub> /SANCH	Cr(VI) / 94.3%	Adsorption/Photocatalysis	Hydrogel	[59]
ZnCoFe <sub>2</sub> O <sub>4</sub> @Chitosan	Tetracycline / 92%	Adsorption	Nanoparticle	[60]
CuO NPs on Carica papaya L.	POME / 66%	Photocatalysis	Peel biowaste/Nanoparticle	[61]
Cellulose/GO/TiO <sub>2</sub>	Methylene blue / 93%	Adsorption/Photocatalysis	Hydrogel	[62]
Polysulfone membranes	Higher flux and rejection	Ultra-filtration	Membranes	[63]
Green ceramic hollow membrane	Oil/water / 99.9%; Oil flux 137.2 L/m <sup>2</sup>	Filtration	Membrane	[64]
BC-Fe/Zn	Water permeance 6.55 ± 0.08 L/m <sup>2</sup> ·h·bar	Filtration	Membrane	[65]
Nutraceutical Industrial Pepper Seed Spent (NIPSS)	Brilliant green / 144.6 mg/g	Adsorption	Nanoparticle	[66]
Ca alginate/TiO <sub>2</sub> fibers	Methyl orange / 90%	Ultra-filtration	Membrane	[67]
Chitosan and alginate composite (CSAL)	Turbidity < 5 NTU; TSS < 20 mg/L	Filtration	Membrane	[68]
Carbon microspheres	Methylene blue /	Adsorption	Poplar	[69]

Green Materials	Pollutant/% Removal/Qmax (mg/g)	Mechanism	Raw Material/Form	Reference
(CSn)	536.64 mg/g		waste/Microspheres	
Corn leaf adsorbent	Malachite green / 91%	Adsorption	Corn leaves	[70]

**Table 3 (Continued): Advanced Green Materials in Water and Wastewater Treatment**

Green Materials	Pollutant/% Removal/Qmax (mg/g)	Mechanism	Raw Material/Form	Reference
Zeolites with thermal activation	Nickel 87%, Copper 99%, Cadmium 99%, Lead 100%	Adsorption	Particle	[71]
Chitosan/carboxymethylcellulose polyelectrolyte complexes	Cd <sup>2+</sup> 98.46%; Pb <sup>2+</sup> 97.14%	Adsorption	Particle	[72]
CuO-NPs on Portulaca oleracea extract	TSS 95.2%; TDS 86.7%; COD 64.4%; BOD 91.4%	Photocatalysis	Nanoparticles	[73]
Bacterial cellulose/γ-(2,3-epoxypropoxy) aerogel	Oil/water separation; Dye adsorption	Adsorption	Aerogel	[74]
TiO <sub>2</sub> -cellulose nanocrystal	Rhodamine B 97%; Methylene blue 97%	Photocatalysis	Aerogel	[75]
Copper sulfide (CuS)	Methylene blue 95%; Rhodamine B 92%	Photocatalysis	Hydrogel	[76]
Grape residues with Azotobacter vinelandii	NPs of 210–240 nm	Photocatalysis	Grape residues/Coal	[77]
Cellulose nanofiber (CNF) membrane	High selectivity and reusability	Filtration	Membrane	[78]
Chitosan/polyaniline nanofibrous composite	Blue dye 113,814.9 mg/g; Orange dye 618.0 mg/g	Filtration	Membrane	[79]
Thin-film nanofibrous composite with barium alginate	Permeation flux 112.5 ± 1.8 L/m <sup>2</sup> ·h; Tensile strength 8.17 MPa	Filtration	Membrane	[80]
CN PFs membrane	Oil-water separation; Photocatalytic degradation	Filtration	Membrane	[81]
Butanediol succinate (PBS)	TOC 95%; Nitrate 95%	Adsorption	Biofilm	[82]
Pistacia soft shell (PSS)	COD 67%; Turbidity 87%	Adsorption	Coal	[83]

**Cellulose nanofibers (CNFs)** are a prime example of nanomaterials derived from natural sources like wood, cotton, and hemp through mechanical, chemical, or enzymatic treatments [41]. Their high aspect ratio confers a large surface area, high tensile strength, and an abundance of surface hydroxyl groups, making them exceptionally valuable for water treatment [40]. Their utility spans the adsorption of heavy metal ions and organic contaminants to serving as foundational building blocks for constructing high-performance filtration membranes [76]. A relevant advancement is the functionalization of CNFs with carboxyl groups, which significantly enhances their adsorption capacity for metals such as lead and cadmium, positioning them as powerful tools for water remediation [39]. Furthermore, integrating CNFs into polymeric matrices results in membranes with superior mechanical properties and enhanced filtration efficiency, considerably expanding their applicability in advanced water treatment systems [6].

**Chitosan**, a linear polysaccharide derived from chitin in crustacean shells and insect exoskeletons, is characterized by its excellent biocompatibility, biodegradability, and notable adsorption capacity [41]. The presence of reactive amino and hydroxyl groups in its structure facilitates effective binding to various contaminants, including heavy metal ions, dyes, and other organic compounds [84]. This biopolymer is widely utilized as an adsorbent, flocculant, or as a key component in composite materials designed to improve water treatment processes [84]. Recent research highlights that chitosan membranes modified with graphene oxide nanoparticles exhibit an outstanding capacity for adsorbing organic contaminants, reinforcing their potential in sophisticated water purification technologies [58, 85]. Similarly, the combination of chitosan with inorganic materials like montmorillonite has enabled the creation of composites with improved mechanical and thermal properties, increasing their durability and viability under demanding operational conditions [86].

In parallel, other **bio-based nanomaterials** such as pectin, lignin, and chitin nanofibers represent sustainable alternatives. Their large specific surface area, inherent biodegradability, and diverse functional groups make them adaptable to various applications, from the selective adsorption of specific contaminants to their incorporation into advanced filtration systems [87]. A highly effective strategy has been the integration of biopolymers like chitosan with clays such as bentonite or kaolinite. This combination creates a synergistic effect, leveraging the large specific surface area of the clays and the functional groups (e.g., amino, hydroxyl) of the biopolymer. This not only significantly increases the number of adsorption sites and strengthens interactions with contaminants but also improves the mechanical stability of the composite and allows for its reuse, enhancing overall efficiency in treating contaminated water [42]. A complementary approach involves combining biopolymers (chitosan, alginate) with synthetic polymers (polyacrylamide, polyvinyl alcohol) to develop hydrogels with superior mechanical and adsorption properties. This merger brings together the biodegradability and biocompatibility of biopolymers with the stability and processability of synthetic polymers, resulting in materials with increased adsorption capacity, controlled swelling behavior, and greater viability for reuse in practical applications [49].

A frontier of innovation involves the **incorporation of metallic nanoparticles** into biopolymer matrices to drastically enhance functionality. For instance, integrating silver nanoparticles into chitosan hydrogels has shown high efficacy in the removal of bacteria and organic contaminants due to the potent antimicrobial properties of silver [50, 94]. Similarly, the addition of zinc oxide nanoparticles to alginate hydrogels has been shown to increase the adsorption capacity for heavy metals and improve the material's performance under adverse environmental conditions, highlighting its potential for advanced water purification [88]. Titanium dioxide ( $TiO_2$ ) nanoparticles incorporated into polymeric matrices have proven highly efficient in the photocatalytic degradation of persistent organic pollutants, reinforcing their utility in environmental remediation [41]. Furthermore, the functionalization of biopolymers with magnetic nanoparticles, such as iron oxide ( $Fe_3O_4$ ), has enabled the development of composite materials with advanced capabilities for easy magnetic separation and recovery after use. These compounds are notable for their enhanced mechanical and chemical stability, which extends their operational lifespan and makes them ideal for continuous wastewater treatment processes [28]. This strategic combination optimizes both the adsorption capacity and practical durability of these materials, consolidating their role as practical and sustainable alternatives.

The integration of biopolymers like cellulose or chitosan with photocatalysts such as  $TiO_2$  or  $ZnO$  has proven highly effective in enhancing the degradation of organic contaminants [12]. This creates a synergistic system where the biopolymer first adsorbs the contaminants, concentrating them near the photocatalytic sites, where they are then efficiently degraded [85]. This synergy results in improved treatment efficiency manifested through faster

degradation kinetics, a reduction in the recombination of photogenerated electron-hole pairs, and greater overall stability of the composite material [84]. Recent research has further explored the functionalization of biopolymers with specific chemical groups to improve their interaction with both the photocatalyst and the target contaminants. This includes tailoring surface chemistry to increase affinity for specific pollutants and enhance electron transfer during the photocatalytic process, generating highly effective composites for remediating water contaminated with a wide spectrum of organic compounds [52, 89].

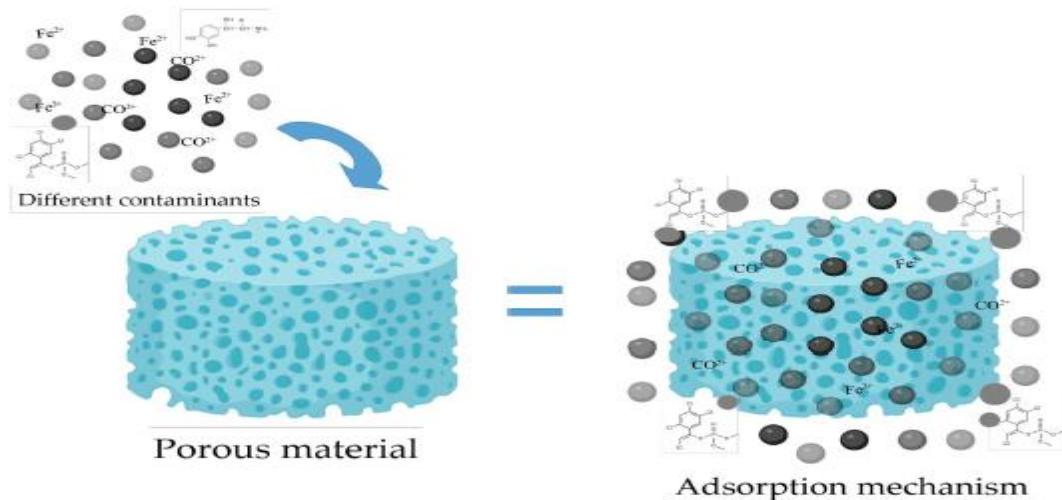
Finally, the **antimicrobial applications** of green nanomaterials are particularly promising for disinfection. Chitosan-based nanomaterials are effective against a wide range of waterborne pathogens (bacteria, fungi, viruses) due to their cationic nature, which disrupts microbial cell walls [90-92]. The potency of silver, a known disinfectant, is greatly amplified when synthesized as nanoparticles due to the enormous increase in surface area-to-volume ratio, enhancing interaction with and neutralization of microorganisms [82, 93, 94]. The integration of these antimicrobial nanoscale agents into biopolymer matrices creates multifunctional composites capable of simultaneous disinfection and adsorption, offering a comprehensive and sustainable approach to ensuring water safety [22, 95].

## 6. Processes and Principles Utilized to Treat Water and Wastewater

The application of green materials in water and wastewater treatment encompasses several fundamental processes and principles that leverage their unique properties for sustainable contaminant removal. Adsorption stands as the most widely researched mechanism, utilizing materials like biochar, chitosan, and cellulose nanofibers to capture pollutants through physical interactions (van der Waals forces, pore filling) and chemical processes (chemisorption, ion exchange, hydrogen bonding) [67,68,70]. These renewable adsorbents demonstrate remarkable efficiency in removing heavy metals, dyes, and emerging contaminants while offering advantages of biodegradability and regeneration potential. Photocatalysis represents another crucial approach, where green-synthesized nanoparticles (e.g., TiO<sub>2</sub>, ZnO, CuO) supported on biopolymer matrices generate reactive oxygen species under light exposure to degrade organic pollutants through oxidation processes [71,73,107]. This mechanism enables effective breakdown of complex contaminants including pharmaceuticals and pesticides, with several studies demonstrating removal efficiencies exceeding 90% under optimized conditions.

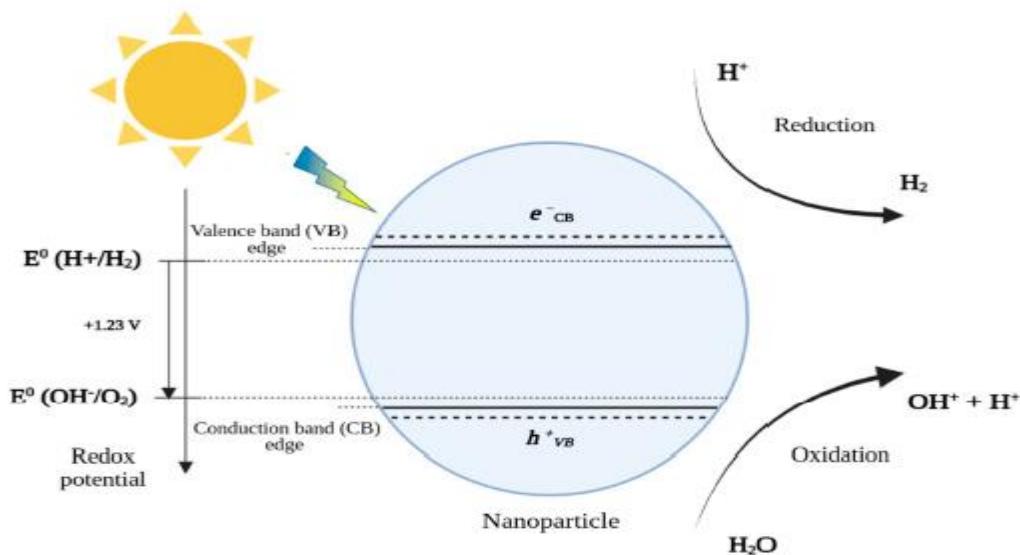
### 6.1. Adsorption

Adsorption is a fundamental and widely researched process in water treatment that involves the accumulation of substances at the interface between a solid adsorbent and a liquid phase. This process is governed by several mechanisms, including physisorption (van der Waals forces), chemisorption (chemical bonding), ion exchange, hydrogen bonding, and  $\pi$ - $\pi$  interactions [67,68,70]. The effectiveness of adsorption depends on the properties of both the adsorbent material and the contaminant, with factors such as surface area, pore size distribution, and functional groups playing crucial roles. Green adsorbents derived from renewable resources—such as biochar from agricultural waste, chitosan from crustacean shells, and cellulose nanofibers from plant biomass—have demonstrated exceptional capabilities in removing heavy metals, dyes, and emerging contaminants. These materials offer sustainable alternatives to conventional adsorbents like activated carbon, aligning with circular economy principles by utilizing waste streams and reducing environmental impact [100].



## 6.2. Photocatalysis

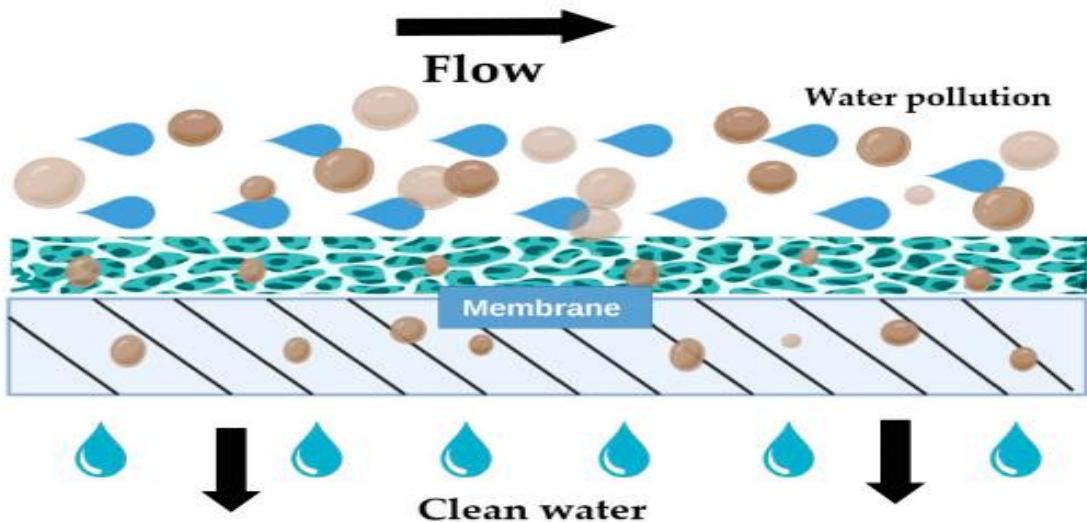
Photocatalysis leverages light energy to drive chemical reactions for pollutant degradation, utilizing photocatalysts such as  $\text{TiO}_2$ ,  $\text{ZnO}$ , and green-synthesized metal nanoparticles supported on biopolymer matrices [71,73]. This process involves the generation of electron-hole pairs upon photoexcitation, leading to the formation of reactive oxygen species (ROS) like hydroxyl radicals ( $\cdot\text{OH}$ ) and superoxide anions ( $\cdot\text{O}_2^-$ ), which oxidize and mineralize organic pollutants. Green photocatalysts, often derived from plant extracts or integrated with biopolymers like chitosan and cellulose, enhance sustainability by reducing reliance on toxic chemicals and energy-intensive synthesis methods. Applications include the degradation of pharmaceuticals, dyes, and pesticides in wastewater, with efficiencies exceeding 90% under optimized conditions [107,108]. The synergy between adsorption and photocatalysis in composite materials further improves treatment performance by concentrating pollutants near active sites [109].



## 6.3. Polymeric Membranes and Filtration

Polymeric membranes are critical for physical separation processes in water treatment, classified based on pore size into microfiltration (MF), ultrafiltration (UF), nanofiltration (NF), and reverse osmosis (RO) [76,79]. Green

membranes, fabricated from biopolymers such as cellulose, chitosan, and alginate, offer biodegradable and renewable alternatives to synthetic polymers. These membranes function by selectively allowing water molecules to pass while retaining contaminants like bacteria, viruses, heavy metals, and organic compounds. Composite membranes, incorporating nanomaterials like graphene oxide or metal nanoparticles, enhance mechanical strength, fouling resistance, and selectivity. For instance, chitosan-based membranes modified with  $\text{TiO}_2$  exhibit improved photocatalytic activity alongside filtration capabilities [77,78]. The development of green membranes aligns with sustainability goals by reducing plastic waste and leveraging natural materials for high-performance water purification.



#### 6.4. Raw Material

The selection of raw materials is pivotal in designing sustainable water treatment technologies. Green materials are typically derived from renewable resources, including agricultural waste (e.g., rice husks, corn stalks), industrial by-products (e.g., lignin from paper pulp), and natural polymers (e.g., chitosan, cellulose) [38,41]. These feedstocks are characterized by their abundance, low cost, and minimal environmental impact. Functionalization through chemical or physical modifications enhances their efficacy—for example, carboxylation of cellulose nanofibers improves metal adsorption, while cross-linking chitosan increases its stability in aqueous environments. The use of raw materials like expired oils for bio-based adsorbents or grape residues for nanoparticle synthesis further exemplifies waste valorization [57,75]. Life cycle assessments (LCAs) are essential to evaluate the sustainability of these materials, ensuring that their production, use, and disposal do not inadvertently exacerbate environmental burdens. By prioritizing renewable and waste-derived resources, green water treatment technologies contribute to resource conservation and circular economy objectives [23,29].

**Table 7: Examples of Raw Materials and Their Applications in Green Water Treatment**

Raw Material	Source	Application	Key Properties/Advantages	Reference
Cellulose nanofibers	Plant biomass (e.g., wood, hemp)	Adsorption, membrane filtration	High surface area, biodegradability	[40,41]
Chitosan	Crustacean shells	Adsorption, coagulation,	Cationic nature, antimicrobial	[35,36]

Raw Material	Source	Application	Key Properties/Advantages	Reference
		membranes		
Biochar	Agricultural waste	Adsorption of metals/organics	Porosity, surface functional groups	[18,19]
Alginate	Brown seaweed	Hydrogel beads, encapsulation	Gel-forming ability, biocompatibility	[42,43]
Plant extracts (e.g., Portulaca oleracea)	Plants	Green synthesis of nanoparticles	Reducing/stabilizing agents	[71,73]
Grape residues	Winery waste	Carbon source for microbial growth	Abundant polysaccharides	[75]
Expired oils	Waste oils	Bio-based adsorbents		

## 7. Modeling Applied to Performance of Green Materials

The performance of green materials in water treatment is increasingly optimized through advanced modeling techniques that predict behavior, efficiency, and scalability. Computational tools, including **Artificial Neural Networks (ANNs)**, **Response Surface Methodology (RSM)**, and **Adaptive Neuro-Fuzzy Inference Systems (ANFIS)**, are employed to simulate adsorption kinetics, photocatalytic degradation, and membrane filtration processes [28,29,60]. These models correlate operational parameters (e.g., pH, temperature, contaminant concentration, material dosage) with removal efficiencies, enabling the design of tailored materials for specific pollutants. For instance, ANNs have been used to predict the adsorption capacity of biochar for heavy metals, while kinetic models (e.g., pseudo-first/second-order) describe reaction rates [99,102]. Thermodynamic modeling further assesses spontaneity ( $\Delta G^\circ < 0$ ) and endothermic/exothermic nature of processes [104]. Machine learning approaches also aid in material selection and synthesis optimization, reducing experimental trials and enhancing reproducibility. Integrating multi-scale modeling—from molecular dynamics (e.g., contaminant-material interactions) to process-level simulations—supports the development of high-performance green materials with precision [118,120].

## 8. Economic Aspects and Sustainability

The adoption of green materials hinges on their economic viability and alignment with sustainability principles. While initial costs for some advanced green materials (e.g., functionalized nanocellulose) may be higher than conventional alternatives, their lifecycle benefits—including **renewable sourcing, reusability, and reduced environmental footprint**—often justify investment [20,65]. Key economic considerations include:

- **Raw Material Costs:** Waste-derived feedstocks (e.g., agricultural residues, shellfish waste) are low-cost or free, minimizing expenses [23,38].

- **Synthesis Efficiency:** Green synthesis routes (e.g., using plant extracts for nanoparticle fabrication) avoid expensive reagents and energy-intensive processes [26,44].
- **Regeneration and Reuse:** Materials like chitosan beads or magnetic biochar can be regenerated multiple times, lowering long-term costs [52,70].
- **Circular Economy Integration:** Valorizing waste streams (e.g., converting biomass into biochar) reduces disposal costs and generates revenue [14,15].

Sustainability is evaluated through **Life Cycle Assessment (LCA)**, which quantifies impacts from raw material extraction to disposal. Green materials typically exhibit lower greenhouse gas emissions, energy consumption, and ecotoxicity compared to synthetic counterparts [66,136]. For example, bioplastics like PLA emit 75% fewer GHGs than conventional plastics [25,26]. However, challenges such as water usage in biopolymer production or land competition for biomass sources require careful management [22,23]. Certifications (e.g., ISO 14040) and policies promoting green procurement further drive adoption, ensuring that economic and environmental benefits are balanced [21,138].

## 9. Challenges and Future Perspectives of Green Materials

Despite significant advancements, green materials face several challenges that must be addressed to enable widespread implementation:

1. **Performance and Durability:** Many green materials lack the mechanical strength, stability, or longevity of synthetic alternatives, especially under harsh industrial conditions [19,20].
2. **Scalability:** Scaling lab-scale synthesis to industrial production while maintaining consistency and cost-effectiveness remains difficult [65,91].
3. **Regeneration and Disposal:** Efficient regeneration protocols for spent adsorbents or photocatalysts are needed, and the environmental impact of degraded nanomaterials requires further study [53,134].
4. **Standardization and Regulation:** Lack of standardized protocols for evaluating green materials and unclear regulatory frameworks hinder commercialization [137,139].

Future perspectives focus on:

- **Advanced Functionalization:** Engineering materials with enhanced properties (e.g., selective adsorption sites, improved photocatalytic activity) via chemical modification or hybrid composites [42,87].
- **AI and Automation:** Leveraging AI for predictive design and automated synthesis to optimize material performance and reduce development time [118,126].
- **Circular Systems:** Developing integrated processes where waste from one application becomes feedstock for another (e.g., using spent adsorbents in construction materials) [14,15].
- **Policy Support:** Governments and industries must incentivize green material adoption through subsidies, carbon credits, and mandates for sustainable water treatment [21,138].

Research priorities include exploring underutilized biomass sources (e.g., algal biomass), improving material stability for reuse, and conducting full LCAs to validate sustainability claims. By addressing these challenges, green materials can become cornerstone technologies for achieving sustainable water management globally [30,31,140].

**Table 8: Key Challenges and Future Directions for Green Materials**

Challenge	Current Status	Future Direction	Examples
<b>Scalability</b>	Lab-scale synthesis dominates	Continuous flow production; modular systems	Pilot plants for nanocellulose production [65]

Challenge	Current Status	Future Direction	Examples
<b>Durability</b>	Limited stability in extreme pH/temperature	Cross-linking; composite reinforcement	Chitosan-montmorillonite composites [85]
<b>Cost</b>	High for some nanomaterials	Waste valorization; energy-efficient synthesis	Biochar from agricultural waste [18]
<b>Regulation</b>	Lack of standardized guidelines	Development of ISO standards for green materials	Certification systems for biodegradability [112]
<b>Environmental Impact</b>	Unknown long-term effects of nanoparticles	Green toxicology assessments; safe-by-desi	

## 10. Conclusions

Green materials represent a transformative paradigm in water and wastewater treatment, offering sustainable solutions to global challenges of pollution and resource scarcity. Derived from renewable resources such as agricultural waste, biopolymers, and plant extracts, these materials leverage mechanisms including adsorption, photocatalysis, and membrane filtration to effectively remove contaminants ranging from heavy metals and dyes to emerging pollutants. Their intrinsic properties—biodegradability, low toxicity, and often lower lifecycle environmental impacts—align with circular economy principles and the United Nations Sustainable Development Goals, particularly SDG 6 (Clean Water and Sanitation).

Advanced modeling techniques, including artificial intelligence and kinetic simulations, have proven invaluable in optimizing the design and application of these materials, enabling precise predictions of performance and scalability. Economically, while initial costs may be higher for some advanced formulations, the use of waste-derived feedstocks, potential for regeneration, and reduced long-term environmental burdens enhance their viability.

However, challenges remain in scalability, durability under operational conditions, regulatory standardization, and comprehensive understanding of environmental impacts. Future efforts must focus on industrial-scale production, integration of hybrid processes, and robust policy frameworks to support adoption.

In conclusion, green materials are not merely alternatives but essential components of next-generation water treatment technologies. Through continued innovation, cross-sector collaboration, and commitment to sustainability, they hold the promise of delivering efficient, equitable, and environmentally responsible water purification for a rapidly evolving world.

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