

Review Article

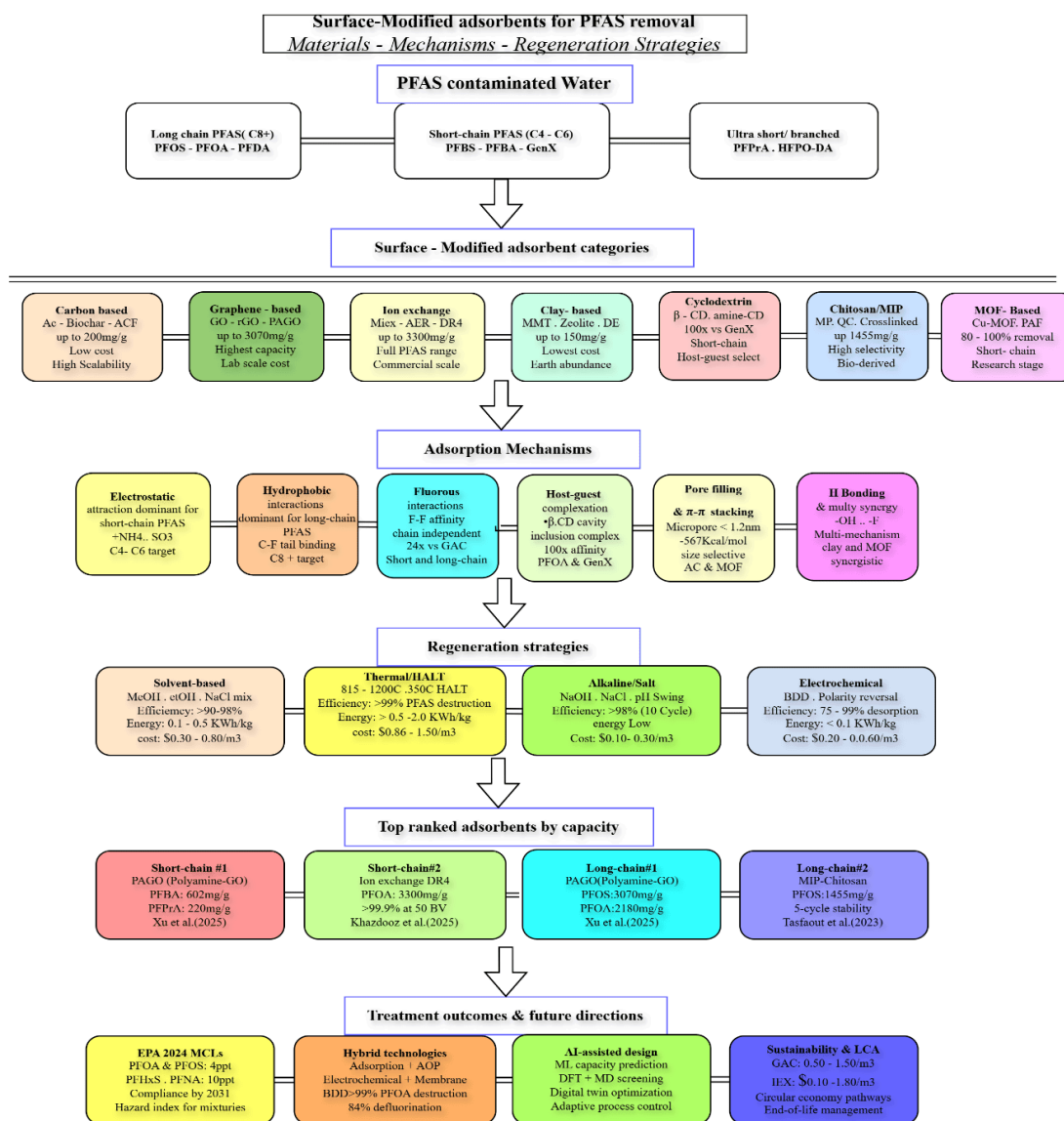
A Comprehensive Review of Surface-Modified Adsorbents for Improving Per- and Polyfluoroalkyl Substances (PFAS) Removal: Materials, Mechanisms, and Regeneration Strategies

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Per- and polyfluoroalkyl substances (PFAS) are persistent organic pollutants that pose significant risks to human health and ecosystems. Adsorption is among the most effective and scalable methods for PFAS removal; however, conventional adsorbents often show limited affinity for short-chain PFAS and reduced efficacy in complex water matrices. Recent advances in surface-modified adsorbents, including functionalized carbons, clays, biopolymers, graphene derivatives, ion exchange resins, cyclodextrin polymers, and metal-organic frameworks (MOFs), have demonstrated enhanced selectivity, adsorption capacity, and regeneration potential. Comparative analyses indicate that graphene-based and MOF materials are particularly promising for short-chain PFAS, while carbonaceous and clay-based adsorbents remain economically viable options for long-chain compounds. Nonetheless, significant knowledge gaps remain regarding long-term stability, regeneration feasibility, and performance validation in real-world settings. The environmental implications of adsorbent disposal also warrant immediate attention, as PFAS-laden materials pose a risk of secondary pollution if not managed through safe end-of-life strategies. Broader frameworks for managing emerging pollutants underscore the need to integrate PFAS remediation with multi-contaminant treatment approaches. Future directions highlight hybrid technologies that combine adsorption with advanced oxidation, electrochemical treatment, and membrane systems. Emerging tools such as artificial intelligence and machine learning can expedite adsorbent design, predict performance, and optimize regeneration cycles. Additionally, techno-economic and sustainability assessments are crucial for translating laboratory findings into scalable, environmentally responsible solutions. By situating PFAS remediation within interdisciplinary contexts, including groundwater risk assessment, principles of the circular economy, and AI-driven innovation, this review offers a critical roadmap for advancing next-generation PFAS cleanup technologies.

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Graphical abstract



Capacity reported under optimized lab conditions. real world performance varies with NOM. Competing anions, and mixed PFAS matrices

#= recommended for that PFAS class. BV= Bed Volume. GAC = Granular Activated Carbon. IEX = ion Exchange Resin

Highlights

- Surface-modified adsorbents exhibit superior PFAS removal efficiency compared to conventional materials.
- Electrostatic, hydrophobic, and fluorous interactions govern enhanced PFAS adsorption performance.
- Comparative evaluation identifies graphene-based and MOF adsorbents as most promising for short-chain PFAS removal.
- Critical knowledge gaps remain in regeneration feasibility, long-term stability, and real-world performance validation.
- Safe end-of-life management of PFAS-loaded adsorbents is essential to prevent secondary pollution risks.
- Integration of adsorption with advanced oxidation, electrochemical treatment, and membrane systems enhances remediation potential.
- Artificial intelligence and machine learning accelerate adsorbent design, performance prediction, and process optimization.
- Techno-economic and sustainability assessments highlight energy demand, resource use, and circular economy pathways.
- Groundwater contamination pathways and risk assessment frameworks are critical for evaluating PFAS migration and exposure.

- Interdisciplinary perspectives connect PFAS remediation with broader emerging pollutant management frameworks.

1. Introduction

Per- and polyfluoroalkyl substances (PFAS) are synthetic persistent organic pollutants, and their worldwide distribution has caused environmental damage and health problems for humans^[1]. PFAS compounds include short chains with fewer than eight carbon atoms and long chains with eight or more carbon atoms^[2]. The long-chain compounds like perfluorooctane sulfonate (PFOS) and perfluorooctanoic acid (PFOA) pose more severe environmental issues than the short-chain compounds^{[3][4]}. PFOS displays stronger hydrophobic properties and greater overall negative charge than PFOA because its perfluoroalkyl chain is longer and includes a sulfonate functional group^[5]. Furthermore, these properties of PFOS enable it to bind more effectively to various sorbent materials^[6]. Previous research has demonstrated that carbon- and mineral-based adsorbents exhibit better removal performance for PFOS and PFOA due to this tendency^{[7][8]}. The sorbent surfaces exhibit better PFOS partitioning due to increased hydrophobicity, and the strong negative charge of PFOS enhances its electrostatic attraction to positively charged sorbents^[9]. The different structural characteristics of PFOS and PFOA help account for the observation that PFOS removal generally occurs more effectively across various sorption mechanisms^[10]. To understand the varied sorption behavior, it is essential first to analyze the molecular architecture of PFAS, characterized by a carbon backbone in which hydrogen atoms are partially or fully replaced by fluorine^[11]. The compound forms a carbon-fluorine bond that is highly polar, with a strength of 485 kJ/mol, thereby enhancing chemical and thermal stability. PFAS materials exhibit both hydrophilic and hydrophobic characteristics because their structure contains a hydrophilic head group and a hydrophobic C-F tail. PFAS materials have become widespread in industrial applications through their use in household products, industrial products, flame retardants, and waterproof clothing, resulting in significant environmental distribution^{[12][13]}. PFAS can bioaccumulate in human and animal bodies, leading to multiple harmful health effects, such as lower birth weights in infants and a higher risk of kidney cancer during adulthood^{[2][14]}.

In light of increasing evidence regarding these health risks, regulatory agencies have begun to set enforceable limits on PFAS in drinking water. The U.S. Environmental Protection Agency (EPA) established its first National Primary Drinking Water Regulation (NPDWR) for PFAS in April 2024 under the Safe Drinking Water Act, in response to growing health risks and widespread environmental contamination. The regulation established Maximum Contaminant Levels (MCLs) of 4 parts per trillion (ppt) for PFOA and PFOS individually, and 10 ppt for perfluorohexane sulfonic acid (PFHxS), perfluorononanoic acid (PFNA), and hexafluoropropylene oxide dimer acid (HFPO-DA, also known as GenX chemicals). A new Hazard Index was established by the rule to control PFAS mixtures of two or more compounds, which produce cumulative health impacts when found together in drinking water. Public water systems must finish their first monitoring by 2027, according to the regulation, while they must reach total compliance by 2031. The regulation requires advanced remediation technologies to achieve ultra-low removal thresholds while efficiently eliminating both long-chain and short-chain PFAS because it uses detection limits that operate at low parts-per-trillion levels^[15].

Meeting these strict regulatory standards has increased demand for advanced, efficient PFAS removal technologies. PFAS remediation technologies operate through two distinct methods: destructive and non-destructive. Destructive technologies break C-F bonds to produce harmless molecules from PFAS. These technologies include chemical oxidation, advanced reduction, electrochemical oxidation, photocatalysis, sonochemical treatment, hydrothermal reaction, plasma treatment, and thermal destruction^[16]. Alongside these physicochemical destructive approaches, biological destruction pathways have attracted growing attention as low-energy, sustainable alternatives. Microbial defluorination, in which microorganisms cleave C-F bonds via reductive, hydrolytic, and oxidative pathways mediated by enzymes such as fluoroacetate dehalogenases, reductive dehalogenases, and cytochrome P450 monooxygenases, offers a promising complement to conventional destructive technologies, particularly under mild operating conditions where energy-intensive physicochemical methods are impractical^[17]. In contrast, non-destructive technologies use physical separation methods to extract PFAS from materials, producing concentrated PFAS products. The non-destructive technologies use three methods: sorption, reverse osmosis, and nanofiltration^[18]. Recent advances in microbial consortia-based remediation have further expanded the toolkit for PFAS transformation: syntrophic microbial communities exploiting co-metabolic networks, metagenomics-guided discovery of novel PFAS-degrading microbes, and integrated bioelectrochemical systems represent promising strategies for in situ biodegradation in soil-groundwater environments^[19].

While each approach offers distinct advantages, the two technologies function as separate methods, but their combination yields optimal PFAS removal. Adsorption has emerged as the top PFAS removal technology because it offers a cost-effective solution that achieves high removal rates while protecting the environment. Previous studies utilized specific adsorbents, including biochars, granular and powdered activated carbon, carbon nanotubes, magnetic biochars, natural clays, metal nanoparticles, soils, and anion exchange resins^[20].

The effectiveness of these adsorbents is not uniform; it varies significantly based on specific material characteristics. PFAS adsorption depends on adsorbent properties, such as surface functional groups, aromaticity, anion exchange capacity, and pore size and pore volume^[21]. PFAS molecules exhibit complex

sorption behavior due to their hydrophilic, hydrophobic, and oleophobic C-F chains. The main driving forces behind PFOA and PFOS adsorption are electrostatic interactions and the hydrophobic effect [22]. Despite these interactions, conventional adsorbents frequently fail to deliver adequate performance under real-world conditions. Scientists modified adsorbents by altering surface morphology or chemical composition because the adsorbents exhibited performance drops when faced with organic matter and water constituents and showed slow sorption rates and reduced capacity to distinguish between different substances [23].

This limitation has driven innovation toward a new generation of engineered materials, such as amine-modified carbonaceous materials, β -cyclodextrin-based polymers, and organic-inorganic hybrid materials [24]. Researchers have studied modified adsorbents extensively, but they have failed to gather all existing evidence into a comprehensive synthesis. To guide this review, three questions were identified: 1) What type of surface modifications are most effective for enhancing the removal of different PFAS classes? 2) What are the dominant mechanisms reported for these enhanced adsorbents? 3) What regeneration strategies have been reported to demonstrate both efficiency and sustainable performance? The review systematically evaluates the available evidence on PFAS removal using surface-modified adsorbents that employ different modification strategies, adsorption mechanisms, and regeneration approaches.

2. Review methodology

This review provides a comprehensive assessment of surface-modified adsorbents for PFAS removal from aqueous solutions. A systematic literature search was conducted using the Web of Science, Scopus, and Google Scholar databases, covering publications from 2008 to 2025. Search terms included combinations of PFAS, PFOA, PFOS, adsorption, surface modification, functionalization, and regeneration. Studies were included if they: 1) reported experimental data on modified adsorbents for PFAS removal, 2) provided quantitative data on adsorption capacity or removal efficiency, and 3) were published in peer-reviewed journals. The research focused on studies examining how modifications alter material properties, their impact on performance, and the potential for material reuse. Additionally, citation tracking and reference list screening were used to identify additional articles containing this information.

3. Conventional adsorbents in PFAS removal: overview

Conventional adsorbents such as activated carbon, ion-exchange resins, biochar, clays, MOFs, chitosan, cyclodextrins, and molecularly imprinted polymers have been investigated for PFAS removal. However, each class shows distinct limitations in selectivity, stability, or regeneration, particularly for short-chain PFAS. As summarized in Table 1, these constraints have motivated extensive surface modification strategies to overcome performance gaps.

A critical analysis of Table 1 highlights that the most significant practical limitations vary considerably among different adsorbent classes and treatment contexts. In the case of activated carbon, the primary real-world limitation is not the surface area; rather, it lies in its limited selectivity for short-chain PFAS (C4 - C6) and the competitive interference from natural organic matter (NOM), which can diminish PFAS adsorption capacity by 30–60% in surface waters. Although ion exchange resins are effective across various chain lengths, their practical constraints stem primarily from NOM fouling and the generation of concentrated brine waste during regeneration. For metal-organic frameworks (MOFs), the principal barriers to deployment remain their aqueous instability and high synthesis costs, despite their remarkable capacities observed in laboratory settings. Biochar and clay-based materials, while abundant and cost-effective, often exhibit inconsistent performance in realistic water matrices and lack adequate selectivity for short-chain PFAS without surface modification. Chitosan and cyclodextrin polymers show strong selectivity through host-guest and electrostatic mechanisms, yet they face challenges related to mechanical stability and pH sensitivity, which restrict their application to controlled conditions. Collectively, these insights suggest that no single conventional adsorbent class can fully address the complete spectrum of PFAS at the part-per-trillion concentrations mandated by the 2024 EPA maximum contaminant levels (MCLs), thereby underscoring the need for the surface modification strategies discussed in Section 4.

Adsorbent	Limitation	Need for Modification
Activated carbon	Limited selectivity for short-chain PFAS ^{[25][26][27]} , competes with natural organic matter ^[28] ; requires frequent regeneration ^[29] ; Decreased efficiency at higher pH ^[20] .	Surface functionalization to enhance selectivity ^{[30][31]} , pore size optimization for short-chain PFAS ^[26] , regeneration methods development ^{[25][29]} , and quaternary ammonium compounds ^[31] .
Ion exchange resins	High cost compared to other compounds ^{[29][25]} , performance affected by competing ions ^[32] , limited capacity for certain PFAS compounds ^[32] , regeneration generates concentrated waste streams ^[33] , and resin fouling by organic matter ^[33] .	Development of PFAS-specific functional groups ^[34] , Hybrid materials to reduce fouling, improved regeneration techniques ^[29] , and enhanced hydrophobic and electrostatic interactions ^[32] .
Biochar	Variable quality based on feedstock, lower adsorption capacity than AC, poor mechanical strength, limited selectivity, insufficient removal of short-chain PFAS ^[3] .	Chemical activation to increase surface area, Metal oxide impregnation ^[35] ^[34] , controlled pyrolysis conditions, and surface modification with quaternary ammonium ^[3] .
Clay minerals	Limited surface area ^[29] , low adsorption capacity for neutral PFAS, poor selectivity in complex water matrices, challenging separation after treatment ^[29] , and interlayer collapse in some conditions ^[24] .	Organo-modification with quaternary ammonium, pillaring to increase interlayer spacing, acid activation to increase surface area, magnetic modification for easier separation ^[29] , and combination with other adsorbents.
Metal-organic frameworks	High production cost ^[29] , poor stability in water ^[29] , challenging scale-up ^[36] , potential metal leaching ^[29] , limited research on long-term stability ^[29] .	Hydrophobic ligand incorporation ^[29] , mixed metal approaches ^[29] , development of water-stable MOFs, Functionalization with fluorophilic groups ^[29] , and integration with other materials for stability ^[26] .
Chitosan-based materials	Limited mechanical strength ^[37] , pH-dependent performance ^[37] , poor stability in acidic conditions ^[37] , low adsorption capacity for some PFAS ^[37] , and degradation over time ^[38] .	Cross-linking to improve stability, grafting with functional groups, Composite formation with other materials, magnetic modification for separation, and development of chitosan-based beads/hydrogels ^[38] .
Graphene and graphene oxide	High production cost ^[39] , difficult separation from water ^[39] , aggregation issues ^[39] , challenging scale-up ^[39] , and limited regeneration potential ^[39] .	Functionalization with amino-groups ^[34] , formation of 3D structures to prevent aggregation, integration with other materials (composite) ^[40] , development of magnetic graphene derivatives ^[41] , and surface modification to increase selectivity ^[39] .
Minerals and mineral oxides	Variable performance based on mineral type, limited surface area for some minerals, sensitivity to solution pH ^[42] , poor selectivity in complex matrices, and low capacity for short-chain PFAS ^[43] .	Surface modification with organic compounds ^[34] , nano-sizing to increase surface area ^[44] , composite formation with carbon materials ^[45] , controlled morphology development, and incorporation of active metal sites ^{[41][46]} .
Molecularly imprinted polymers	Complex synthesis process ^[47] , high production cost, limited binding sites, template leaching concerns, less effective for structurally diverse PFAS ^[25] .	Optimization of template monomer interactions, development of universal PFAS recognition sites, integration with other materials for enhanced stability, scale-up of production methods, and improvement of regeneration techniques ^[25] .
Carbon nanotubes	Extremely high cost, potential environmental risk, challenging dispersion in water, difficulty in recovery after use, and limited adsorption capacity for some PFAS ^[48] .	Surface functionalization to increase hydrophobicity, development of CNT-polymer composites, magnetic modification for easier separation, oxidation to increase surface functionality, and creation of hierarchical structures ^[48] ^[49] .
Cyclodextrin-based materials	High cost for pure cyclodextrins ^[50] , limited stability in extreme pH ^[50] , relatively small cavity size for longer PFAS, water solubility challenges, and lower capacity than some conventional adsorbents ^[51] .	Polymer cross-linking to improve stability ^[52] , functionalization to enhance selectivity, development of cyclodextrin-based networks, integration with other materials, optimization of cavity size for different PFAS ^[49] .

Table 1. Limitations of conventional adsorbents and modification strategies

4. Mechanism and regeneration of enhanced adsorbents

4.1. Surface Modification Strategies

Surface modification is a promising technique for overcoming the limitations of conventional adsorbents. Notably, this part summarizes the major modification approaches for various material classes to improve PFAS removal.

4.1.1. Modified carbonaceous materials for PFAS removal

Biochar modification

A 2021 study by J. Steigerwald explored using spent coffee grounds (SCG) as a cost-effective adsorbent for PFOS removal from water. Converting SCG to biochar with potassium hydroxide (KOH) created SCGKOH, boosting surface area and making it 300 times more efficient than untreated pyrolyzed SCG. Untreated pyrolyzed SCG had low PFOS adsorption, but KOH activation achieved up to 99.6% removal. The optimal SCG/KOH ratio was 1:1, with a max adsorption capacity of 43.4 mg/g. SCGKOH's high efficiency, surface area, negative charge, and low surface groups indicate high carbon content. Its structure and hydrophobic regions enable PFOS adsorption via hydrophobic binding through the CF chain, despite limited surface functionality. Overall, activated waste enhances trace-level PFOS removal^[53]. A 2023 study by I. Militao et al. found that rice straw biochar and Moringa oleifera seed albumin in alginate beads effectively adsorbed PFOS and PFBS from water. Albumin beads removed 87% PFOS and biochar 99% in 16 hours; biochar also removed 40% PFBS in under 48 hours, outperforming other natural adsorbents. pH and organic matter had little effect, with hydrophobic interactions dominating over electrostatic ones^[54]. Across biochar modifications, KOH activation and biopolymer encapsulation both enhance PFOS removal substantially, with hydrophobic interactions consistently identified as the primary driving force.

Carbons modifications

In 2016, Y. Zhi et al. increased activated carbon's basicity to evaluate its PFOS and PFOA removal. They treated carbons from coal, coconut shell, wood, and phenolic polymers with heat and ammonia. Results showed ammonia treatment was more effective, with higher point-zero charge and basicity improving adsorption. Effectiveness varied by material; wood-based carbon and fibers showed 1-3 orders of magnitude enhancement, while some materials had reduced PFOS/PFOA uptake^[51]. In 2017, W. Chen et al. prepared polyacrylonitrile fiber (PANF) and activated carbon fibers (PACF) for water purification, showing PACFs had higher sorption capacities for PFOS and PFOA than PANF, outperforming commercial activated carbons. TACFs' efficiency is due to more sorption sites. Studies show multilayer adsorption occurs after the monolayer via electrostatic and hydrophobic mechanisms, forming micelle-like structures. Spent PACFs can be regenerated and reused over multiple cycles, offering a notable advantage^[55]. Together, these studies show that surface basicity enhancement and fiber-based architectures consistently improve carbonaceous adsorbent performance for long-chain PFAS through hydrophobic and electrostatic mechanisms, while regenerability remains a key practical advantage.

Carbon nanotube modification

In several studies, mechanisms such as hydrophobicity (which also leads to hemimicelle/micelle formation), electrostatics, and hydrogen bonding are the primary mechanisms of removal by activated carbon adsorbents. These mechanisms depend on the source material of the activated carbon, surface chemistry, and the type of carbon used^[48]. However, in 2018, L. Liu and colleagues grafted different metal nanoparticles (iron, copper, and zinc) onto multiwalled carbon nanotubes (MWCNTs) to remove PFOA. This facilitates the removal of PFOA via inner-sphere complexation, hydrophobic interactions, and electrostatic mechanisms between PFOA and the modified MWCNT surfaces^[56].

Graphene-based materials

Pervez et al. (2024) studied eight GO-based adsorbents for removing PFAS from river water. GO modified with cetyltrimethylammonium chloride (GO-CTAC) was most effective, removing nearly 100% of all 11 PFAS, including short- and long-chain types. Adsorption followed a pseudo-second-order model, indicating rapid chemisorption, with the Toth isotherm fitting equilibrium data, reflecting complex surface interactions. GO-CTAC's positive surface charges enhanced electrostatic attraction and hydrophobic interactions with PFAS, overcoming issues like aggregation and low affinity. These results highlight surface charge engineering's role, with GO-CTAC showing promise for effective PFAS cleanup, especially under challenging conditions^[40]. Xu et al. (2025) introduced PAGO, a highly charged, monodisperse 2D adsorbent created by attaching 1-nm polyamine layers to graphene oxide (GO) nanosheets. PAGO's PFAS capacity (~3,070 mg/g) surpasses unmodified GO and activated carbon, making it one of the best graphene-based adsorbents. It achieves 57-95% of its capacity within a minute and nearly 100% PFAS removal in minutes. The study shows strong adsorption from electrostatic attraction, hydrogen bonding, and hydrophobic

interactions. The adsorbent can be regenerated, and PFAS destroyed, supporting a closed-loop treatment. These results position PAGO as a next-gen material overcoming common GO limitations^[57]. Research by T. Wu et al. shows that PFOS adsorbs onto few-layered porous graphite (FPG) through electrostatic and hydrophobic mechanisms. PFOS intercalates between FPG lamellae and may penetrate hydrophobic pores on the surface. This dual binding model explains FPG's high multilayer PFOS capacity^[58]. Across graphene-based modifications, surface charge engineering via cationic functionalization is the most consistent predictor of high PFAS removal efficiency, particularly for short-chain compounds that challenge purely hydrophobic adsorbents.

4.1.2. Natural and bio-derived materials

Clay minerals modification

M. Wang et al. (2021) studied the best adsorbent for PFAS removal: modified montmorillonite clay with carnitine and choline versus unmodified clay. They used experiments and modeling to optimize interactions and predict efficacy. They found that hydrogen bonding, hydrophobic, and electrostatic interactions greatly improved PFOA and PFOS binding. PFOA bonded via its carboxyl group to modified clay and its fluorinated tail to interlayers. PFOS mainly bonds through hydrogen bonds between its sulfonate group and hydroxyl groups on the organic amendment^[13]. Du et al. (2016) developed a new adsorbent, fluorinated montmorillonite (F-MT), by replacing cationic surfactants with fluorinated ones. F-MT effectively removes PFOS and PFOA, surpassing activated carbon and resin. It can be fully regenerated with methanol and reused for five cycles without performance loss. F-MT selectively adsorbs PFOS and PFOA even amid other organics, due to binding with its fluorinated chains, while hydrocarbons adsorb different organics. This enhances understanding of PFAS adsorption mechanisms on fluorinated adsorbents^[59]. Khodabakhshloo and Biswas developed oleylamine-modified composites from Iranian zeolite and diatomaceous earth (DE) for PFOS removal from simulated wastewater. Characterization via TGA, SEM, FTIR, and surface/pore size analysis confirmed successful surface modification. The modified materials showed much higher PFOS adsorption capacities: oleylamine-zeolite reached 25.5 mg/g versus 0.39 mg/g for raw zeolite, and oleylamine-diatomite reached 14.1 mg/g versus 4.72 mg/g for raw DE. Adsorption modeling indicated monolayer binding, with performance improvements due mainly to electrostatic and hydrophobic interactions^[23].

Dong et al. (2021) created a modified natural clay with imidazolium ILs to absorb PFOS and PFOA, achieving max capacities of 66.2 mg/g for PFOA and 151.5 mg/g for PFOS. The adsorbent was regenerated with over 98% efficiency using three eluents: 50 mM NaCl, 500 mM NaCl, or a 50/50 methanol/water mix^[24].

Mineral oxide modification

A 2020 study by M. Hassan et al. examined red mud-modified sawdust (RMSDN600) and unmodified sawdust (SDN600) in removing PFAS from water. RMSDN600, containing minerals like magnetite (Fe₃O₄), ferrihydrite, and desilicated minerals, was tested against SDN600. The adsorption relies on hydrophobic interactions, stronger than PFOS-PFOS electrostatic repulsion. The maximum capacities were 194.6 mg/g for RMSDN600 and 178.6 mg/g for SDN600 at pH 3.1. The higher capacity of RMSDN600 results from protonated metal groups and a more ordered graphitic carbon structure from the catalytic degradation of cellulose and hemicellulose^[21].

4.1.3. Polymer-based modifications

Chitosan-based materials

In 2008, Q. Yu made a chitosan-based molecularly imprinted polymer (MIP) with epichlorohydrin crosslinker and PFOS as a template. It has a high PFOS adsorption of 560 μ mol/g, surpassing that of a non-imprinted polymer (258 μ mol/g). The MIP exhibits good selectivity with little interference from other anionic pollutants. Electrostatic interactions are crucial for PFOS sorption. It can be regenerated and reused at least five times without losing performance^[60]. S. Deng et al. (2012) grafted long polymer brushes with quaternary ammonium groups onto cotton via surface-initiated ATRP. The modified cotton adsorbed PFOS and PFOA, reaching equilibrium in 4-12 hours. At pH 5, capacities were 3.3 mmol/g for PFOS and 3.1 mmol/g for PFOA, surpassing most adsorbents. Adsorption was effective across pH 3-10, with quaternary ammonium groups enabling removal through anion exchange. A. Yang et al. (2020) discovered that amino groups added to cyclodextrin (β -CD) polymer crosslinkers improve binding of anionic PFAS. They compared tripodal crosslinkers with amino and amido groups, finding that amino crosslinkers were more effective at PFAS removal. Both β -CD polymers outperformed activated carbon in removing PFOA, demonstrating the importance of host-guest complexes. The amino polymer showed excellent affinity for GenX, while amido adsorbents had low binding. The amine- β -CD polymer exhibited 100 times higher affinity for PFOA compared to GenX, indicating the challenges of removing short-chain PFAS. Overall, amino-functionalized β -CD polymers are promising for targeting resistant short-chain PFAS. ^[9]

Cyclodextrin-based polymer

A. Yang et al. (2020) found that amino-functionalized cyclodextrin (β -CD) crosslinkers enhance the binding of anionic PFAS. They prepared adsorbents using tripodal crosslinkers with amino or amido groups for comparison. The study revealed that amino crosslinkers are more effective than amido ones in removing PFAS. Both β -CD polymers outperformed activated carbon in PFOA removal due to host-guest complex formation. While amido adsorbents showed low GenX binding, the amino polymer exhibited high affinity for GenX, driven by electrostatic interactions. The amine- β -CD polymer had a 100-fold higher affinity for PFOA compared to GenX, indicating that short-chain PFAS like GenX are more challenging to remove. Overall, amine-functionalized β -CD polymers are promising candidates for targeting short-chain PFAS, which resist conventional adsorbents^[51].

4.1.4. MOF-based materials

Recent advances highlight the potential of metal-organic frameworks (MOFs) for PFAS remediation. A review by Lee et al. (2025) notes that MOFs utilize various adsorption mechanisms such as electrostatic attraction and hydrogen bonding to enhance selectivity for short-chain PFAS. However, challenges remain in aqueous stability, regeneration, and scalability, emphasizing the need for rationally designed functionalized MOFs. An experimental study in Small (2025) introduced a bio-derived, water-stable MOF, $\text{CuII}_2(\text{S}, \text{S})\text{-his} \times 5\text{H}_2\text{O}$, which achieved 80–100% removal of long-chain PFAS and up to 86% for short-chain PFAS with rapid adsorption kinetics and excellent reusability. Structural analysis confirmed specific binding modes between PFAS and the MOF, underscoring their promising attributes while highlighting the need for ongoing innovation to address stability and scalability.^{[61][62]}

4.1.5. Ion exchange resin functionalization

Based on previous studies, ion exchange resins remove long-chain PFAS via hydrophobic interactions and hydrogen bonding, whereas short-chain PFAS rely more on electrostatic interactions ^{[36][63]}. Furthermore, S. Woodard et al. (2017) found that anion exchange resins can effectively eliminate PFAS via two mechanisms: dual ion exchange and adsorption. This is due to the characteristics of PFAS with a hydrophobic nonionic carbon tail and a negatively charged head, and the resin beads containing neutral copolymers with positive sites. Consequently, the PFAS tail attaches to the hydrophobic resin backbone, and the head bonds to the positive sites. This dual mechanism of ion exchange and adsorption enables higher PFAS removal than with solely adsorption media ^[64].

A cross-comparative assessment of the modification strategies reviewed in Sections (4.1.1 – 4.1.5) reveals several critical inconsistencies and knowledge gaps that warrant explicit synthesis. First, reported adsorption capacities vary by orders of magnitude across studies, even within the same adsorbent class, largely because experiments use different initial PFAS concentrations, pH levels, ionic strengths, and water matrices. For example, modified biochar capacities for PFOS range from 43.4 mg/g (SCGKOH, Steigerwald et al., 2021) to 194.6 mg/g (red mud-modified sawdust, Hassan et al., 2020), making direct comparisons unreliable without standardized protocols. Second, most studies in this section used synthetic single-compound solutions, which systematically overestimate performance relative to real-world matrices containing NOM, competing ions, and mixed PFAS. Third, for short-chain PFAS (C4–C6), consistent high-performance modification strategies remain scarce: only cationic modifications (quaternary ammonium, polyamine layers) and fluorine-functionalized materials demonstrate reliable removal, whereas carbon-based and clay-based modifications largely fail below C6. Fourth, regeneration feasibility is underreported across all modification categories; fewer than half the studies reviewed provide multi-cycle regeneration data, and most test only two to five cycles under idealized conditions, leaving long-term stability poorly characterized. These gaps collectively indicate that the field has prioritized initial capacity optimization over practical performance validation, and that future comparative studies should adopt standardized PFAS mixtures, environmentally relevant water matrices, and extended cycling protocols to generate data suitable for technology selection decisions.

4.2. Adsorption mechanisms

The results of earlier research indicate that adsorbent surface modifications enhance PFAS removal through multiple mechanisms. The design process for optimized adsorbents targeting specific PFAS compounds requires an understanding of these mechanisms.

4.2.1. Electrostatic Interactions

PFAS compounds maintain their anionic state at typical environmental pH levels because of their low acid dissociation constant (pK_a) properties^[55]. PFAS removal through electrostatic interactions achieves its highest efficiency. The process of surface modification by introducing a positive charge, achieved via quaternization with quaternary ammonium groups or amino-functionalization, results in stronger electrostatic attraction between the adsorbent material and the anionic PFAS headgroups.

Two short-chain PFAS examples most clearly demonstrate the importance of electrostatic interactions in this section. First of all, Yang et al. (2020) showed that amino-crosslinked β -CD polymers outperformed amido-functionalized variants specifically for short-chain and branched PFAS (GenX), because

electrostatic interactions from the amino groups compensate for the diminished hydrophobic driving force at shorter chain lengths^[65]. Secondly, Data S et al. (2025) confirmed this pattern using quaternary-ammonium-grafted flax fibers, which were designed and validated specifically to target short-chain PFAS through strong electrostatic attraction. Together, these studies establish electrostatic attraction as the dominant mechanism for short-chain PFAS removal, in contrast to the hydrophobic-driven uptake of long-chain compounds^[66].

The 2016 study by Zhi et al. showed that cotton treated with quaternary ammonium groups achieved PFOS/PFOA removal primarily through anion exchange^[31]. Moreover, the research of Yang et al. (2020) demonstrated that amino-crosslinked cyclodextrin polymers outperformed amido-functionalized variants because electrostatic interactions enabled better removal of short-chain and branched PFAS^[51]. Electrostatic interactions were the key factor enabling PFOS detection during chitosan-based MIP adsorption experiments, as confirmed by the study by Yu et al. (2008)^[60]. In addition, the dual mechanism of ion exchange resins occurs because PFAS, being negatively charged, bind to positive sites on neutral copolymer beads. At the same time, its hydrophobic tail attaches to the resin backbone, according to Ateia et al. (2019)^[26].

The electrostatic mechanism is particularly important for removing short-chain PFAS. Electrostatic attraction increases in strength with decreasing PFAS chain length because it compensates for diminished hydrophobic interactions in short-chain compounds, according to Lei et al. (2023)^[67].

Finally, cationic adsorbents demonstrate outstanding performance for PFBA and PFBS, which are difficult to adsorb with standard activated carbon materials, according to this research.

4.2.2. Hydrophobic Interactions

Hydrophobic interactions between the perfluorinated carbon tail of PFAS and the hydrophobic regions of adsorbents primarily drive adsorption processes. This mechanism is effective for removing long-chain PFAS because these substances exhibit greater hydrophobicity than their shorter counterparts^[24]. Steigerwald et al. demonstrated in 2021 that SCGKOH could efficiently adsorb PFOS via hydrophobic interactions with its carbon-fluorine chain because the material lacked surface functional groups^[23]. According to the research conducted by Militao et al. (2023), hydrophobic interaction served as the primary mechanism for PFOS removal from biochar, while electrostatic interaction functioned as a secondary mechanism^[54]. Chen et al. (2017) studied multilayer adsorption via electrostatic and hydrophobic interactions, leading to micelle-like structures that formed on PACF surfaces^[52]. The research conducted by Hassan et al. (2020) demonstrates that adsorbent surfaces exhibit stronger hydrophobic interactions that govern adsorption than PFOS-PFOS electrostatic repulsion between PFOS molecules^[21]. Recent computational studies have provided molecular-level insights into hydrophobic interactions. Lei et al. (2023) demonstrated that PFAS molecules prefer to align their long hydrophobic perfluoroalkyl chains with graphite-like aromatic structures on biochar surfaces, resulting in binding energies that increase with chain length^[67]. The study explains that hydrophobic interactions remain the main mechanism for long-chain PFAS adsorption on carbon-based materials, as organic matter competes with this process. The extent of hydrophobic interactions depends on the length of the PFAS chains. Hydrophobic binding is more effective for longer chains because shorter chains rely on electrostatic interactions for removal^[51]. The research conducted by Minervino et al. (2024) demonstrated that hydrophobic interactions are the main mechanism by which both anionic and zwitterionic PFAS bind to carbon-based materials, based on their systematic studies of zwitterionic PFAS^[68].

Hydrophobic interactions are notably weaker for short-chain PFAS (e.g., PFBS, PFBA, GenX) due to their shorter fluorocarbon chains. The reduced number of -CF₂- units lowers the hydrophobic surface area, leading to decreased adsorption affinities. Ateia et al. (2019) highlighted this chain-length dependence, showing that both adsorption capacity and removal efficiency sharply decline for PFAS with fewer than six carbons on conventional hydrophobic adsorbents^[69]. Furthermore, Gagliano et al. (2020) similarly demonstrated that granular activated carbon, which performs well for PFOS and PFOA via hydrophobic adsorption, shows substantially reduced effectiveness for short-chain homologs, underscoring the need for surface modifications that introduce complementary electrostatic or host-guest mechanisms when targeting this PFAS subset^[70].

4.2.3. Fluorous Interactions

Fluorous interactions, which describe how fluorinated compounds interact more strongly with one another than with other materials, are a specialized method for removing PFAS from contaminated sites. This study by Du et al. (2016) demonstrated that fluorinated montmorillonite (F-MT) could effectively bind PFOS and PFOA via its hydro-oleophobic fluorinated chains that exhibit fluorous affinity. In contrast, other organic pollutants could only attach to the hydrocarbon regions of the material^[59].

Fluorous interactions are based on the unique electronic properties of the carbon-fluorine bond, which has high polarizability and the lowest surface energy among organic groups. This leads to perfluorinated domains having minimal van der Waals affinity for water and hydrocarbons, while strongly attracting each other. When a perfluorinated adsorbent meets the fluorocarbon tail of a PFAS molecule, they associate through enhanced London dispersion forces,

driven by the collective polarizability of C-F dipoles. This selectivity remains effective for short-chain PFAS, like PFBS and PFBA, due to fluorine-fluorine complementarity rather than the molecule's hydrophobic surface area. Du et al. (2016) explicitly demonstrated this chain-length-independent selectivity by showing that F-MT adsorbs PFAS via fluororous affinity while excluding hydrocarbon pollutants entirely, a result that would be impossible with a purely hydrophobic mechanism. Several more recent studies confirm and extend the importance of fluororous interactions in PFAS removal^[71]. He et al. (2024) demonstrated that porous aromatic frameworks functionalized with both electrostatic and fluororous segments achieved a 24.1-fold improvement over activated carbon for PFOA removal, and explicitly concluded that fluororous interactions represent the most effective single mechanism for short-chain PFAS removal, outperforming both hydrophobic and electrostatic mechanisms individually when chain length decreases^[72]. Xu et al. (2025) provided additional evidence at the graphene oxide platform: their PAGO material, which combines polyamine adlayers with graphene oxide, explicitly included fluorine-fluorine (F-F) interactions among its multi-mechanism binding array alongside electrostatic attraction and hydrogen bonding, and achieved removal capacities of up to 3,070 mg/g across a broad range of PFAS chain lengths including short-chain compounds such as PFBA^[52]. In the MOF literature, Lee et al. (2025) highlight that incorporating fluorophilic ligands into MOF frameworks specifically enhances short-chain PFAS removal by creating fluorine-rich pore environments that attract PFAS fluorocarbon tails through fluororous affinity, a design principle now recognized as essential for next-generation adsorbents targeting the short-chain PFAS that regulatory limits now require to be controlled at parts-per-trillion concentrations. Taken together, these findings position fluororous interactions not as a niche mechanism but as a central design principle for adsorbents intended to remove the spectrum of PFAS chain lengths, with particular relevance for short-chain compounds (PFBS, PFBA, GenX) that are increasingly regulated but remain resistant to conventional hydrophobic adsorbents^[61].

4.2.4. π - π Interactions

The π - π stacking mechanisms, though less commonly discussed in the PFAS literature than in other organic pollutant literature, can contribute to adsorption on aromatic carbon surfaces and graphene-based materials. Aromatic adsorbents attract PFAS aromatic moieties via their π -electron systems, thereby creating this interaction. Studies showed that graphene oxide and reduced graphene oxide materials with higher π -electron density can adsorb more organic contaminants via π - π stacking. The electron-withdrawing nature of fluorine atoms can influence the π -electron distribution, potentially altering PFAS adsorption system interactions^{[3][24]}.

4.2.5. Pore-Filling Mechanisms

Pore-filling is known as a critical physical adsorption mechanism, particularly for microporous adsorbents. The size-selective nature of this mechanism makes it especially important for targeting specific PFAS chain lengths.

The study conducted by Kebede et al. (2025) showed that ball-milled colloidal activated carbon (CACBM) achieved better PFAS removal because its pore-filling mechanism moved to a more efficient stage. The Polanyi-Dubinin-Manes (PDM) isotherm model demonstrated that micropore-filling was the main mechanism, as CACBM achieved 7.4× better PFOS extraction and 6× better PFOA extraction than granular activated carbon^[23]. The relationship between pore size and PFAS adsorption has been systematically investigated. Furthermore, the research by Liu Z et al. (2024) established that ultra-micropores with dimensions less than 1.2 nm serve as the primary PFOA adsorption sites because they exhibit higher adsorption efficiency than small mesopores, which have dimensions in the 2.0-3.0 nm range. The molecular dynamics simulations showed that PFOA molecules bind to pore walls in ultra-micropores with maximum interaction energies of $-567.32 \text{ kcal}\cdot\text{mol}^{-1}$ because the overlapping potential barriers from both sides of the pore walls create more effective adsorption sites. PFOA forms micelles and hemi-micelles in small mesopores, which enables these pores to serve as both transport pathways and effective adsorption sites^[24]. Moreover, the thermodynamic analysis by Wang et al. (2024) established that PFOA adsorption on biochar proceeds through spontaneous physical pore-filling, and Gibbs free energy changes (ΔG°) show a range between -2.24 and -5.38 kJ/mol ^[25].

However, the physical nature of pore-filling also means that desorption can occur relatively easily when environmental conditions change, highlighting the importance of considering both adsorption and desorption characteristics in remediation applications.

4.2.6. Hydrogen Bonding

Hydrogen bonding contributes to PFAS adsorption through interactions between functional groups on the adsorbent and PFAS molecules. Hydrogen bonds can form between COOH and OH groups on adsorbents and oxygen atoms in PFAS anions. Fluorine atoms can also form hydrogen bonds with the OH groups of adsorbents^[14]. Wang et al. (2021) showed that hydrogen bonding increased the binding strength of PFOA and PFOS to modified clays. PFOA formed hydrogen bonds between its carboxyl group and functional groups on clay carnitine, while PFOS bonded through hydrogen bonds between its sulfonate group and hydroxyls on organic amendments^[13]. The studies indicate that the methyl group C-H bonds create hydrophobic interactions with PFOS, whereas the carbonyl groups C=O enable hydrogen bonding^[54].

4.2.7. Host-Guest Complexation

The materials that scientists create from cyclodextrin use their ability to form host-guest inclusion complexes as a special method for achieving adsorption. The cyclodextrin types, including α , β , and γ , all possess hydrophobic inner cavities that can form protective shields around PFAS molecules, while β -cyclodextrin is the most effective because its cavity size matches the dimensions of multiple PFAS substances. The research conducted by Yang et al. (2020) demonstrated that both crosslinker functions and interactions with the β -CD guest molecule determine PFAS binding strength. The combined effects of electrostatic interactions arising from amino crosslinkers and the host-guest binding mechanism produced strong binding and high capacity; the amine-modified β -CD polymer demonstrated an affinity for PFOA that was 100 times that of GenX [51]. Choudhary et al. (2022) used molecular dynamics simulations to show how cyclodextrin interacts with PFAS using mechanistic details. The computational studies demonstrated that the adsorption mechanism comprises two components that operate in parallel: electrostatic attraction between protonated amino groups and the anionic PFAS headgroup, and hydrophobic interactions between the fluorinated tail and the cyclodextrin cavity. The superior performance of amino-functionalized cyclodextrin polymers stems from their binding mechanism, which is more effective than that of single-mechanism adsorbents [76].

4.2.8. Inner-Sphere Complexation and Ligand Exchange

Metal-modified adsorbents remove PFAS by forming inner-sphere complexation bonds. Metal nanoparticle-grafted MWCNTs removed PFOA via inner-sphere complexation, hydrophobic interactions, and electrostatic attraction, according to research by Liu et al. (2018) [56].

In their 2014 research study, Zhang and colleagues discovered that PFOS binds with kaolinite through an initial rapid outer-sphere complex bond, which later transforms into a slow ligand exchange process that removes adsorbed H_2O . PFOS chemisorption to clay mineral surfaces occurs through specific bonding with sulfonate groups to hydroxyl groups while also allowing hydrophobic and electrostatic forces to bind nonspecifically. Researchers have established that effective adsorbent design requires multiple interaction mechanisms to function properly [77]. Recent research has emphasized the importance of designing adsorbents that integrate multiple interaction mechanisms. For example, in their study, He Y. et al. (2024) established that the combination of hydrophobic, fluorine, and electrostatic segments achieves optimal sorption capacity. The electrostatically modified porous aromatic frameworks showed 14.8 times improved PFOA adsorption performance compared to the non-quaternized parent material and 24.1 times better performance than activated carbons. The study found that commercial adsorbents (GAC and ion exchange resins) use hydrophobic and electrostatic interactions as their main removal mechanisms. In contrast, fluorine interactions have emerged as the most effective technique for short-chain PFAS removal [72]. Finally, scientists now recognize computational modeling as a valuable tool for studying how different mechanisms work together. The DFT calculations, together with molecular dynamics simulations, show that effective PFAS adsorbents function by simultaneously engaging multiple binding sites. In contrast, their binding performance depends on the solution chemistry, pH, ionic strength, and the presence of competing organic matter [12][13].

4.2.9. Multi-Mechanism Synergy

The majority of enhanced adsorbents function by employing several combined mechanisms that operate simultaneously. As confirmation, the study by Wu et al. (2018) showed that multilayer PFOS sorption on few-layered porous graphite (FPG) occurs through electrostatic attraction and hydrophobic interactions, as PFOS inserts between hydrophobic lamellae via intercalation and hydrophobic pores on the particle surface [58].

To conclude, the mechanism contributions depend on adsorbent attributes, including surface charge and functional groups, hydrophobicity and pore structure, and PFAS molecular weight, head group, and molecular structure. The next generation of adsorbents needs to be designed through research into the mechanisms that govern interactions among different materials.

Adsorbent class	Modification strategy	PFAS compound	Capacity before(mg/g)	Capacity after(mg/g)	Enhancement factor	Key mechanisms	References
Activated carbon	Ball milling (physical modification)	PFOA, PFOS, PFBA, PFBS	Not explicitly quantified GAC removal (12% for PFOA, 0% for PFOS)	Colloidal Activated Carbon (CAC _{BM}) removal: Up to 89% for PFOS, 73% for PFOA, 55% for PFBS, 30% for PFBA	7.4x for PFOS and 6x for PFOA (based on removal %)	Increased surface area and microporosity; enhanced dispersion; electrostatic and hydrophobic interactions; intraparticle diffusion	[73][78]
Biochar	Magnetic modification (Fe ₂ O ₃ nanoparticles, -100 nm, pre-pyrolysis at 200°C)	PFOS	-20–30mg/g (unmodified sugarcane bagasse BC at 200°C)	120.44 ± 12.37 mg/g	4–6x	Electrostatic interaction, ion exchange, hydrophilic groups, hemimicelle formation, pore filling, bilayer formation	[79]
	Post-pyrolysis thermal treatment (air oxidation at 400°C for 30 min)	PFBS	17–34 (various feedstocks at 800°C, 1st saturation)	40–170 (after 400°C treatment)	2–5x	Increased SSA and porosity, oxidative removal of tarry deposits, increased C/O and C/H ratios (enhanced hydrophobicity)	[80]
Clay minerals	Surfactant-modified montmorillonite (CTAC)	PFUnA, PFBS, PFHxA, PFHpA, PFOA, PFOS, PFNA, PFDA, GenX, PFHxS	-5–10	-40–50	-5–8x	Hydrophobic surface creation; ion exchange; interlayer expansion	[81]
Chitosan	Surface quaternization (chemical modification)	PFOS; PFOA	PFOS: 12.3 mg/g, PFOA: 10.1 mg/g	PFOS: 38.7 mg/g, PFOA: 32.4 mg/g	-3.1x for PFOS, -3.2x for PFOA	Enhanced electrostatic attraction, increased surface charge density, improved hydrophilicity, and regenerability	[82][83]
MOFs	Post-synthetic modification (PSM) vs preassembled (PAM)	PFOA	493 (PAM)	783 (PSM)	1.59x	Increased pore accessibility; Lewis acid–base interactions; electrostatic attraction	[84]
Graphene oxides	Cationic surfactant grafting (GO-CTAC); polyamine adlayer coating (PAGO); amine functionalization (EA, DETA, HMT)	PFBA, PFBS, PFHxA, PFHpA, PFOA, PFOS, PFNA, PFDA, GenX, 6.2 FTSA, PFPrA	GO baseline: 50–90% removal after 48 h; adsorption capacity -75 mg/g (PFOA)	GO-CTAC: -100% removal for 11 PFAS in 1 h; PAGO: 2180–3070 mg/g (PFOA/PFOS), 602 mg/g (PFBA), 220 mg/g (PFPrA)	GO-CTAC: -10× faster kinetics; PAGO: 30–40× capacity increase vs GO	Electrostatic attraction (quaternary ammonium or protonated amines), hydrophobic interactions, hydrogen bonding, F–F interactions	[40][57]
Ion exchange resins	Quaternary ammonium functionalization (MIEX® GOLD); cross-linked DADMAC/BisAAM polymer beads (DR4); porogen-enhanced porosity; strong-base anion exchange	PFBA, PFBS, PFHxA, PFHxS, PFOA, PFOS	MIEX® GOLD: >99% removal at 1 ppm; capacity -1.01–1.05 g/g (PFHxS, PFOA)	DR4: 3300 mg/g (PFOA); MIEX® GOLD: 1.01–1.05 g/g; >99.9% removal for all PFAS at 50 BV	DR4: -30× higher than commercial resins; MIEX® GOLD: -10× higher than many AERs	Strong electrostatic attraction; ion exchange with Cl ⁻ ; hydrogen bonding (DR4); hydrophobic interactions	[85][86]

Adsorbent class	Modification strategy	PFAS compound	Capacity before(mg/g)	Capacity after(mg/g)	Enhancement factor	Key mechanisms	References
Cyclodextrin polymer	Covalent grafting to graphene oxide (GO-Poly-BCD); crosslinking with benzyl chloride, HDI, or EPI	PFBA, PFPeA, PFHxS, PFHpA, PFOA, PFOS, PFDA, PFUDA, PFOSA, N-MeFOSAA, N-EtFOSAA	GO baseline: -1.3 µg/g; β-CD-EPI/HDI: -10-20% removal; β-CD-Cl: up to 75% PFOA	GO-Poly-BCD: up to 4.0 µg/g; β-CD-Cl: log Ka up to 3.3 L/g	~3× (GO-Poly-BCD vs GO); ~2-6× (β-CD-Cl vs β-CD-EPI/HDI)	Hydrophobic interactions, van der Waals forces, host-guest inclusion, electrostatic attraction (amine groups)	[87][88]
Molecular Imprinted Polymer	Electropolymerization of o-phenylenediamine (o-PD) with PFOS template on hydrophobic gold;bulk/surface imprinting using AAM, TFMAA, 4-VPy, chitosan, or DADMAC-based matrices	PFOS, PFOA, PFHxS, PFNA, PFTeDA	NIP baseline: <1-5 mg/g	PFOS: up to 1455 mg/g; PFOA: 5.4-12.4 mg/g	-10× to >1000×	Selective cavity recognition; electrostatic attraction (PFAS anion ↔ protonated monomers); hydrogen bonding; fluorophilic and hydrophobic interactions; surface imprinting enhances accessibility	[89][90]

Table 2. Performance Enhancement Through Surface Modification

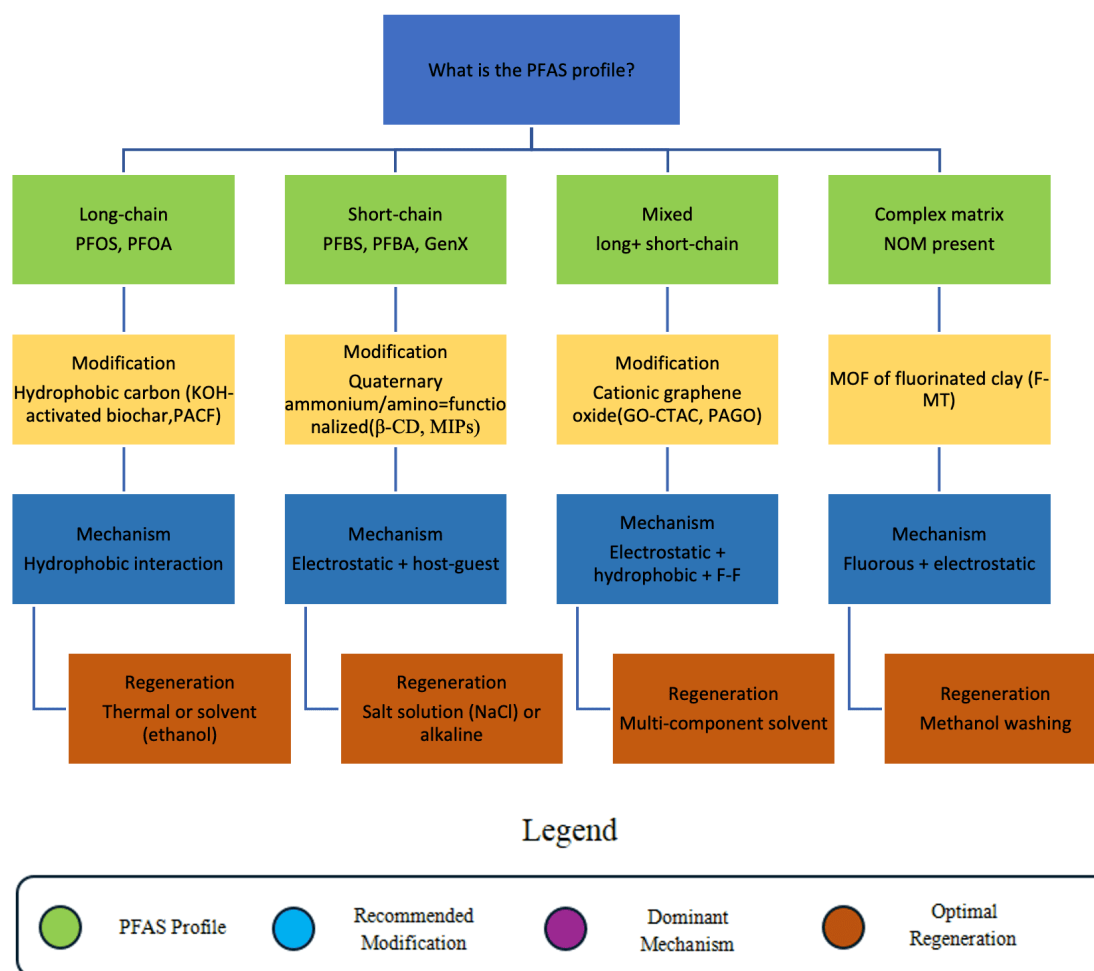


Figure 1. Adsorbent Selection Framework for PFAS Removal Based on Contaminant Profile

4.3. Regeneration and Reusability

The ideal regeneration technique enables complete PFAS recovery via desorption while restoring the adsorbent's capacity for PFAS adsorption without damaging its physical or surface properties. Therefore, the development of optimized regeneration strategies is a fundamental requirement for operational PFAS adsorption systems. Furthermore, surface modifications enhance an adsorbent's initial adsorption capacity, but they also affect the effectiveness of regeneration processes and the durability of adsorbents across multiple usage cycles. The selection of a modification method establishes the primary binding pathways and the most effective regeneration procedure; therefore, combining modification design with regeneration planning becomes essential for real-world implementation^{[2][21]}.

4.3.1. Role of surface modification on regeneration performance

Surface modifications in PFAS remediation work to improve adsorption capacity but create obstacles to regeneration processes. Modified adsorbents, which rely on strong electrostatic interactions through quaternized materials and amino-functionalized polymers, require different regeneration methods from those that rely on hydrophobic interactions. Recent studies show that the characteristics and strength of surface functional groups determine both the energy required for desorption and the success of regeneration^{[3][24]}.

For instance, adsorption materials modified with quaternary ammonium groups require salt solutions or pH-swing methods to break electrostatic bonds for efficient regeneration. Fluorinated modifications, which use organic solvents to break fluorine-fluorine interactions, require specific regeneration methods that must be known for designing effective PFAS treatment systems^{[12][13]}. The regeneration process for modified biochar and activated carbon materials improves structural integrity because their modified forms provide superior mechanical stability compared to their unmodified counterparts^[16]. The

adsorbent's ability to withstand extreme regeneration conditions depends on the specific modification method used. Covalent modifications via grafted polymers and chemically bound functional groups provide greater resistance to regeneration cycles than electrostatically bound surfactants, which lose some material during regeneration ^[83].

4.3.2. Solvent-Based Regeneration

In several studies, researchers have employed methods to regenerate organic solvents during PFAS desorption. In 2021, Dong et al. achieved >98% desorption efficiency for imidazolium IL-modified clay using a methanol/water (50%/50%) mixture ^[24]. Du et al. (2016) showed that fluorinated montmorillonite (F-MT) could be completely regenerated through methanol washing, enabling five consecutive performance cycles without any decrease in efficiency ^[59]. In their 2018 study, Wu et al. achieved 85.3% regeneration efficiency for few-layered porous graphite using 50% ethanol at 40°C for 12 hours ^[58]. In addition, multi-component solvent systems have been identified as the most effective chemical regeneration approach in several recent comprehensive reviews, achieving >90% desorption efficiency compared to single-component solvents (12.5%), salt solutions (2.34%), or alkaline/acidic solutions (1.17%) ^[92]. The enhanced efficiency of multi-component systems is due to their capacity to concurrently disrupt multiple binding mechanisms that regulate PFAS adsorption on modified adsorbents ^[93]. For modified adsorbents, the organic solvent concentration and composition must be optimized based on the modification type. As confirmation, the study by Kashani et al. (2025) showed that quaternized chitosan hydrogels achieved more than 98% PFAS desorption over 10 cycles when tested with dilute NaCl solutions at 0.025 M because their surface-modification design reduced the need for chemical regeneration ^[83]. In contrast, Chaudhary et al. (2024) developed a stepwise methanol-acid regeneration train that operated by desorbing PFAS and co-adsorbed heavy metals from wood-derived biochar through two distinct processes, resulting in more than 90 percent pollutant recovery while allowing adsorbent reuse for three complete cycles ^[94].

Mixed solvent systems that combine organic solvents with salts exhibit enhanced regeneration. To confirm this, in 2021, Liu et al. conducted research in which a 1:1 (v/v) ethanol-1 mmol/L Na₂SO₄ mixed solution was used for Cu/F-rGa regeneration ^[12]. In general, the combined action of organic solvent molecules, which disrupt hydrophobic interactions, together with salt ions, which enable ion exchange, creates a synergistic effect in mixed solvents. The ion exchange process requires this dual-modification feature in adsorbents because both hydrophobic and charged surface groups are present.

4.3.3. Alkaline Regeneration

In the regeneration process, alkaline solutions are known to disrupt electrostatic binding and facilitate PFAS desorption. Yu et al. (2008) showed that chitosan-based MIP adsorbents retained their ability to remove PFOS at full capacity through five adsorption-regeneration cycles, which used a 0.5 M NaOH/acetone (90/10, v/v) mixture at 40°C for 24 hours. The alkaline regeneration process destroyed chitosan's electrostatic binding but enabled complete regeneration without loss of performance ^[60].

The effectiveness of alkaline regeneration is particularly pronounced for adsorbents modified with amine or amino groups, where pH adjustment can protonate/deprotonate functional groups to reverse electrostatic attractions. However, excessive alkalinity or prolonged exposure can damage certain modifications, particularly those involving ester linkages or acid-labile crosslinks.

Based on previous work, it has been concluded that alkaline regeneration is most effective with adsorbents modified with amine or amino groups because pH changes enable functional groups to switch between their protonated and deprotonated states, thereby canceling electrostatic binding.

Furthermore, the research by Yang et al. (2020) demonstrated that amino-crosslinked β -cyclodextrin polymers preserved 89% of their original capacity after 6 cycles using a methanol/water (70/30) mixture. The polymers exhibited greater stability under conditions resembling harsh alkaline environments ^[51].

4.3.4. Salt Solution Regeneration

In salt solutions, high ionic strength can effectively desorb PFAS via ion-exchange mechanisms. Dong and co-workers (2021) demonstrated that both 50 mM and 500 mM NaCl solutions achieved over 98% desorption efficiency for ionic-liquid-modified adsorbents ^[24]. The optimal salt concentration depends on the strength of PFAS-adsorbent interactions. Salt-based regeneration works best for ion-exchange resins and quaternized materials, which bind PFAS via electrostatic interactions. Zhang et al. (2024) showed that quaternary ammonium-modified porous organic polymers with structural tunability achieved 90% PFAS removal efficiency after 5 regeneration cycles using a 10% NaCl-30% methanol mixture. The modification process improved both adsorption capacity and regeneration efficiency compared to unmodified polymers ^[93].

Surface modification plays a critical role in salt regeneration. The adsorption of heavily quaternized adsorbents requires stronger salt solutions and extended contact times because their electrostatic interactions with salts are stronger than those of less heavily quaternized adsorbents. Thus, the optimal salt concentration represents a trade-off between desorption efficiency and the preservation of the modification layer's structure ^{[16][18]}.

4.3.5. Thermal Regeneration

High-temperature treatment is an effective method for the complete regeneration of adsorbents, as it decomposes adsorbed PFAS compounds.

Wu et al. (2018) achieved 99.8% regeneration efficiency by heating the exhausted few-layered porous graphite to 800°C [58]. However, the process requires significant energy resources due to the degradation of the adsorbent material after multiple usage cycles. To address this challenge, scientists have developed advanced thermal regeneration techniques that create specific temperature profiles that effectively break down PFAS while preserving the material's integrity. Thermal reactivation processes carried out at designated treatment centers, operating between 815 and 1200 degrees Celsius, can achieve over 99 percent elimination of PFAS contamination. However, these high temperatures can result in a 10 to 20 percent weight reduction of activated carbon and may alter its surface chemical properties. Additionally, modified adsorbents with organic functional groups attached via grafting are particularly susceptible to thermal degradation, as their modification layer begins to disintegrate at temperatures exceeding 400 degrees Celsius [22]. In addition, the implementation of temperature-control systems on thermally reactivated GAC significantly reduces its environmental impact over its lifespan compared with single-use GAC and regenerable ion-exchange systems. Operating at lower temperatures, starting at 815 degrees Celsius, reduces energy requirements while still achieving effective regeneration. The sustainability benefits of this system hinge on two primary factors: the transportation distance of materials to centralized reactivation plants and the frequency of regeneration processes [95]. In addition to adsorption, thermal processes like pyrolysis are gaining attention for the management of PFAS. McNamara et al. (2023) found that the pyrolysis of biosolids can result in the transportation and transformation of PFAS into py-liquid fractions. This raises concerns about the potential for secondary contamination and underscores the need to combine adsorption methods with destructive technologies to guarantee the complete removal of PFAS [26].

4.3.6. Hydrothermal Alkaline Treatment (HALT)

The hydrothermal alkaline treatment (HALT) regeneration technology offers an innovative solution for effectively removing PFAS contamination while simultaneously restoring adsorbent materials. This method employs a strong alkali and operates at near-critical conditions (e.g., 350°C, 16.5 MPa, 1 M NaOH) to achieve complete PFAS mineralization. A study conducted by Soker et al. in 2023 demonstrated that HALT resulted in over 99% destruction of PFOS adsorbed by granular activated carbon, achieving a defluorination rate of $96 \pm 4\%$ with no fluoroorganic intermediates detected. Additionally, the process operates at significantly lower temperatures than conventional thermal regeneration (350°C versus 815–1200°C), resulting in energy savings while providing the dual benefits of PFAS destruction and adsorbent regeneration [27].

The thermal and chemical stability of surface modifications under alkaline hydrothermal conditions determines how HALT works for modified adsorbents. Carbon-based adsorbents exhibit good HALT tolerance, although their organic polymer, surfactant, and metal nanoparticle modifications will undergo partial degradation during the treatment. Research is needed to evaluate how different modification strategies interact with HALT to identify the optimal combination of modification and regeneration methods [21][22].

4.3.7. Electrochemical Regeneration

Electrochemical methods provide an effective means to regenerate adsorbents by restoring their operational capacity. Liu et al. (2021) demonstrated electrosorption-desorption of Cu/F-rGa by applying a reverse voltage, yielding a 75.5% desorption efficiency [12]. This method enables direct regeneration without introducing chemical substances into the system. The method demonstrates promise as an efficient regeneration solution that requires less than 1 kWh per regeneration cycle, uses only a few chemical reagents, and enables in situ regeneration. The process requires either anodic or cathodic polarization to change surface charge or create reactive materials that support PFAS desorption. Electro-regeneration achieves optimal performance when used with modified adsorbents containing conductive materials, such as metal nanoparticles and graphene. Recent studies have investigated electro-regeneration for PFAS-contaminated adsorbents and found that ion-exchange resins and electroconductive carbon materials achieved the greatest success. The technique works best on modified adsorbents with surface charges that can be adjusted electrochemically. The method requires non-conducting modifications to achieve its full functionality, while co-contaminants pose obstacles to electrochemical methods [98]. The process of coupled electrochemical degradation purifies PFAS contaminants in regeneration brine through an integrated system. Researchers achieved over 99% PFOA degradation using boron-doped diamond electrodes within 3 hours, with 84% defluorination. This method enables researchers to eliminate PFAS contamination in concentrated regeneration waste streams through waste treatment [23][34].

Recent progress in electrochemical treatment highlights the importance of water quality and dissolved organic matter in influencing how PFAS is removed. For instance, Ryan et al. (2025) showed that peroxi-electrocoagulation can effectively reduce PFAS levels, but natural organic matter greatly changes the removal process, emphasizing the necessity for adsorbent designs suited to actual water conditions [99]. Pilot-scale studies underscore the significance of operational optimization in improving treatment efficiency. Govindan et al. (2025) employed response surface methodology to evaluate the electrocoagulation

treatment of greywater, demonstrating that optimized operating conditions can markedly improve PFAS removal while concurrently decreasing energy consumption. This research offers valuable insights for the scalable implementation of adsorption–electrochemical hybrid systems^[100].

4.3.8. Regeneration Efficiency and Cycling Stability

Multiple studies have demonstrated excellent cycling stability for modified adsorbents:

MIP adsorbents: Maintained full capacity over five cycles^[60]. Molecular imprinting ensures that binding sites remain structurally intact through multiple regeneration cycles, with 98.3% regeneration efficiency using NaOH/acetone mixtures^{[25][26]}.

Fluorinated montmorillonite: No performance reduction over five cycles^[59]. The covalent bonding of fluorinated chains to clay surfaces provides exceptional stability, allowing complete regeneration with simple methanol washing^[26].

PACF: Effective regeneration and reuse over multiple cycles^[55]. Polyacrylonitrile-based activated carbon fibers maintain structural integrity during solvent regeneration, though capacity gradually decreases to ~85% by the fourth cycle^[28].

Few-layered porous graphite: High regeneration efficiency maintained^[58]. Both thermal (99.8% at 800°C) and solvent-based (85.3% with 50% ethanol) regeneration methods prove effective, with the thermal method showing superior but more energy-intensive results^[21].

Quaternized chitosan hydrogels: Maintained >98% performance over 10 cycles using a dilute 0.025 M NaCl solution, demonstrating the exceptional regenerability of properly designed cationic modifications^[83].

Amino-crosslinked β -CD polymers: Retained 89% capacity after 6 cycles with methanol/water (70/30) regeneration, showing the good long-term stability of host-guest complexation systems^[51].

Porous organic polymers (POPs): Maintained 90% PFAS removal through 5 cycles using 10% NaCl + 30% methanol, demonstrating that rigid polymer frameworks preserve structure better than flexible materials^[22].

Wood-derived biochar: Achieved >90% pollutant recovery for at least 3 cycles using stepwise methanol-acid regeneration, though capacity gradually declined due to irreversible pore blocking^[24].

Graphene oxide-CTAC: Rapid adsorption kinetics (~30 minutes) were maintained through multiple cycles, though regeneration efficiency declined from 95% (1st cycle) to 78% (5th cycle) due to gradual surfactant loss^[40].

4.3.9. Impact of Surface Modification on Long-Term Stability

The stability of surface modifications during regeneration processes is essential for modified adsorbents to maintain long-term performance across multiple adsorption-regeneration cycles. The stability of modifications depends on several essential factors, which include:

Chemical Stability: Covalently grafted modifications (e.g., ATRP-grafted polymers, silanized surfaces) demonstrate superior stability compared to physically adsorbed modifications (e.g., surfactant coatings). Kashani et al. (2025) demonstrated that covalently cross-linked quaternized chitosan retained 98% of its original capacity after 10 cycles. In contrast, clays with physically adsorbed surfactants typically experience a 10–20 percent capacity loss after 5 cycles due to ongoing surfactant desorption during regeneration^[29].

Thermal Stability: Organic modifications become incompatible with high-temperature regeneration, which exceeds 400°C. Metal oxide modifications and fluorinated surfaces exhibit better thermal stability. Still, even these materials may undergo phase changes and sintering when exposed to standard thermal reactivation temperatures, which range from 815 to 1200°C^{[20][31]}.

Mechanical Stability: The handling and regeneration processes that follow ball-milling create abrasive conditions that degrade the physical properties of all modified materials. The handling of ball-milled activated carbon yields better regeneration performance than granular forms because this process creates more favorable mass-transfer conditions and reduces diffusion limitations^[23].

Structural Integrity: Porous structures face risks of damage through their exposure to extreme conditions during regeneration processes. Research findings demonstrate that activated carbon micropore volume declines by 5% to 15% after five regeneration cycles. In contrast, modified carbons exhibit better preservation, with only 8% to 12% loss because their modification layers provide structural strength^[32].

4.3.10. Sustainability and Techno-Economic Considerations

The efficiency of PFAS remediation systems depends on their ability to remove pollutants, the energy required for regeneration and chemical use, the production of resulting waste, and their overall environmental effects throughout their operational life.

Energy Consumption: Thermal regeneration requires substantial energy, as it uses between 0.5 and 2.0 kilowatt-hours to process 1 kilogram of adsorbent. Chemical regeneration requires between 0.1 and 0.5 kilowatt-hours to process 1 kilogram of material, including solvent recovery. The electro-regeneration process requires the least energy, requiring less than 0.1 kilowatt-hour to produce 1 kilogram of output. The technology is not yet advanced enough for commercial use, and its current state of development makes it difficult to operate [95].

Chemical Requirements: The twelve-solvent system operates as a multi-component system, achieving more than 90% efficiency but generating waste streams that require treatment or disposal. The environmental burden of regeneration chemicals can offset the benefits of extended adsorbent life. The sustainability of modified adsorbents using salt-based regeneration systems can be enhanced because their chemical toxicity impacts are reduced, while their waste treatment becomes easier to manage [24].

Life-Cycle Analysis: The life-cycle assessment results indicate that regenerable ion exchange resins cause less environmental harm than single-use granular activated carbon. The thermal reactivation process requires GAC to operate within its optimal temperature range while also recycling its materials to achieve sustainability results that match or exceed the environmental impact of traditional methods. The environmental impact of modified adsorbents needs to be assessed by examining how their production process affects the performance of their regeneration system and their total operational lifespan [95].

Cost-Effectiveness: An economic analysis shows that regeneration is cost-effective when adsorbents reach their third to fifth cycle limits, with less than 20% performance degradation. The initial price of modified adsorbents becomes competitive when their regeneration efficiency exceeds 85% across multiple usage periods. The break-even point depends on adsorbent cost, regeneration method, PFAS concentrations, and treatment volume [28].

Standardized Cost Benchmarks: Published life-cycle cost analyses provide standardized economic benchmarks that allow direct comparison across technologies [23][101]. Granular activated carbon (GAC) is the lowest-cost adsorbent material at approximately \$0.050-2.00 per kilogram, but its single-use cost at centralized thermal reactivation facilities translates to treatment costs in the range of \$0.50-1.50 per m³ of treated water, depending on PFAS influent concentration, throughput volume, and transport distance to reactivation plants [33][102]. Ion exchange resins carry a significantly higher material cost of approximately \$5-15 per kilogram, yet their ability to regenerate on-site with salt solutions and their longer service life before replacement often result in comparable or lower full lifecycle treatment costs of \$0.10-0.80 per m³ [33][102]. Thermal regeneration of GAC at centralized facilities costs approximately \$0.86-1.50 per m³ treated, reflecting energy-intensive reactivation at 815-1200 °C combined with material losses of 10-20% per cycle and transportation overhead [33][103]. Chemical solvent regeneration of modified adsorbents reduces this to approximately \$0.30-0.80 per m³ [104], while salt-based regeneration of modified adsorbents reduces this to approximately \$0.10-0.30 per m³ when regenerant solutions are recovered and recycled. Electrochemical regeneration, though the most energy-efficient approach at less than 0.1 kWh per kilogram, remains at pilot scale with treatment costs not yet benchmarked at full scale; current estimates suggest a potential range of \$0.20-0.60 per m³, but these figures require validation under operational conditions [105]. These cost differentials underscore that the optimal technology selection requires balancing adsorbent material cost, regeneration energy, chemical inputs, waste disposal requirements, and regulatory compliance thresholds, a multi-criteria trade-off that differs substantially between large municipal systems and small-scale point-of-use applications [101].

4.3.11. Challenges and Future Directions

The field of PFAS adsorbent regeneration has made substantial progress, but it still faces multiple obstacles.

Incomplete Desorption: The optimized regeneration process fails to recover complete capacity because certain PFAS molecules form permanent bonds with the material. This situation becomes most serious when materials undergo strong electrostatic or chemical-bonding modifications. The research path to solving this problem requires scientists to investigate pulsed regeneration methods and sequential multi-stage regeneration systems [48].

Modification Loss: The aggressive regeneration process will result in the removal of some physical modifications that require remodification over time. The research field is currently investigating the development of self-healing modification technology as its next focal point [49].

Co-contaminant Interference: Real-world PFAS applications require treating complex mixtures containing both organic and inorganic contaminants. Regeneration strategies need to develop either selective desorption methods or systems for treating mixed waste materials. The stepwise regeneration technique shows potential for the successful separation of different contaminant groups [106].

Scale-Up Challenges: The majority of regeneration research uses synthetic waters, which researchers test at bench scale. Full-scale and pilot demonstrations are necessary because they establish real-world regeneration performance through testing with flow-through columns, variable water quality, and extended operation lasting over 100 cycles ^[107].

PFAS Destruction in Regeneration: Regeneration reduces PFAS material to smaller volumes, which makes disposal or destruction more difficult. The combination of advanced oxidation, electrochemical degradation, and HALT systems leads to complete PFAS mineralization, thereby completing the treatment process ^{[51][53]}.

Regulatory Compliance: The regeneration processes must comply with hazardous waste handling regulations that protect worker safety and govern the discharge of regeneration waste streams. The use of modified adsorbents requires additional regulatory oversight when modification chemicals or byproducts pose toxicological risks ^[54].

The selection of a regeneration technique depends on the specific adsorbent used, the characteristics of PFAS substances, the costs involved, and the resulting environmental effects. Research must develop regeneration methods that achieve sustainability and cost efficiency while producing minimal secondary waste and sustaining adsorbent function during extended cycling periods. Furthermore, the process of developing new adsorbent materials requires designers to include all regeneration methods in their initial design work rather than treating them as a later consideration. The most effective PFAS remediation systems will use a comprehensive design that integrates modification chemistry, adsorption mechanisms, and regeneration methods, thereby enhancing performance, sustainability, and economic viability throughout the adsorbent material's entire lifespan ^{[31][55]}.

Biological and Hybrid Degradation Pathways: Beyond the physicochemical and adsorption-based strategies reviewed above, emerging biological approaches offer complementary and potentially synergistic pathways for PFAS degradation that deserve critical attention within any comprehensive remediation framework. Fungal-mediated biotransformation represents one of the most promising of these alternatives. Khan & Murphy (2023) demonstrated that *Cunninghamella elegans*, a well-studied metabolic fungus with high cytochrome P450 (CYP) activity, completely consumed 6:2 fluorotelomer alcohol (6:2 FTOH) within 48 hours at a faster rate than previously reported for other fungi, yielding primarily 5:3 fluorotelomer carboxylic acid (5:3 FTCA) as the main metabolite^[108]. Critically, when 1-aminobenzotriazole (a CYP inhibitor) was added, biotransformation was completely abolished, confirming that cytochrome P450 enzymes are the catalytic drivers of this pathway. However, the same study revealed an important mechanistic limitation: the accumulated 5:3 FTCA product inhibits CYP activity in subsequent cycles, which explains why complete mineralization is not achieved by the fungal treatment alone and represents a key challenge for scaling this approach. This mechanistic bottleneck directly motivates the hybrid treatment strategy reported by Khan et al. (2023), which sequentially coupled bismuth oxyiodide (BiOI) photocatalysis with *C. elegans* fungal treatment for PFOA degradation^[109]. Applied individually, each treatment achieved only 35 - 40% PFOA degradation with 20 - 30% defluorination over 3 - 48 hours. However, the sequential combination of photocatalysis first, then fungal exposure, raised overall degradation to 90% with 60% defluorination. The mechanistic explanation is instructive: photocatalytic pre-treatment breaks PFOA down into short-chain perfluorocarboxylic acids without generating the inhibitory 5:3 FTCA intermediate, thereby removing the CYP inhibitor before the fungal stage and allowing the fungus to degrade the remaining substrate more completely. This interaction between photocatalytic and biological mechanisms illustrates a broader principle relevant to adsorption-based systems: sequential or hybrid treatment trains can overcome the individual limitations of each technology when the product profile of one step is compatible with the operational requirements of the next. From an adsorption perspective, fungal pre-treatment could plausibly reduce the concentration and structural diversity of long-chain PFAS entering an adsorbent bed, lowering the mass load, extending service life, and converting recalcitrant precursors into shorter-chain products. However, it must be acknowledged that these shorter-chain transformation products may themselves be more difficult to capture on conventional hydrophobic adsorbents, reinforcing the need for surface-modified or electrostatic adsorbents of the type reviewed in Section 4.1. Integrating biological pre-treatment with engineered adsorption polishing steps therefore represents a promising yet underexplored research direction that could substantially reduce the total cost and chemical footprint of PFAS remediation systems beyond what adsorption alone can achieve.

The collective findings emphasize the necessity of integrating adsorption with complementary destructive technologies. The combination of adsorbents with electrochemical treatments (Ryan et al., 2025), the careful monitoring of transformation risks during thermal processes (McNamara et al., 2023), and the implementation of optimization frameworks for pilot-scale systems (Govindan et al., 2025) will be essential for advancing next-generation PFAS remediation strategies.

Adsorbent type	Modification	Regeneration method	Efficiency (%)	Cycles tested	Capacity retention	References
Quaternary nitrogen	Quaternary nitrogen-grafted activated carbon (SNQ)	Ethanol	65	–	73%	[110]
Quaternary Ammonium Flax Fibers	Poly (METAC) grafting via ATRP	MeOH/ 1% NaCl solution	>78% PFBS >97% PFBA	1	>85% after 1 cycle	[111]
MIP-Chitosan	Molecular imprinting	NaOH/acetone (90/10)	98.3	7	95% after 7 cycles	[60]
Porous Organic Polymer (POP)	Structurally, tunable quaternary ammonium	10% NaCl + 30% methanol	90%	5	90% PFAS removal maintained through 5 cycles	[93]
Graphene oxides(rGO)	Reduced graphene oxide-modified zinc ferrite-immobilized chitosan beads (rGO-ZF@CB)	0.1 M ethanol	80.35	5	Slightly altered	[112]
β -CD polymer	Amine cross-linked	Methanol/water (70/30)	93.6	6	89% after 6 cycles	[113]
Surface-modified quaternized chitosan hydrogels (MQCGs)	Surface-modified bio-based hydrogels derived from cross-linked quaternized chitosan (MQCGs)	0.025 M NaCl solution	>98%	10	Performance maintained >98%	[83]

Table 3. Regeneration Methods for Surface-Modified Adsorbents

4.4. Future Research Directions: Integration with Advanced Technologies

The preceding review of surface-modified adsorbents demonstrates substantial progress in PFAS removal performance. However, meeting the 2024 EPA MCLs of 4 ppt for PFOA/PFOS and 10 ppt for short-chain compounds across the full spectrum of PFAS classes in real-world matrices will require not only improved adsorbent materials but also integration of adsorption with complementary treatment technologies and the application of advanced computational tools for material design and process optimization. This section outlines four priority research directions that represent the frontier of next-generation PFAS remediation.

4.4.1. Integration of Adsorption with Advanced Oxidation Processes (AOPs)

Advanced oxidation processes (AOPs) generate highly reactive species (hydroxyl radicals, sulfate radicals, hydrated electrons) capable of cleaving the C-F bond in PFAS, achieving mineralization rather than concentration. The combination of adsorption and AOP in sequential or simultaneous configurations addresses a fundamental limitation of adsorption-only systems: PFAS removal from the water phase but accumulation in a concentrated waste stream. Integrated AOP-adsorption systems aim to use the adsorbent both as a separation tool and as a support for in-situ PFAS destruction.

Photocatalytic AOP combined with adsorption has been explored using TiO₂-modified graphene oxide composites, which concentrate PFAS near the photocatalytic surface while UV irradiation generates reactive radicals for defluorination. **Mabaso et al. (2024)** demonstrated that photocatalytic membrane reactors combining TiO₂ with GO-based membranes achieved simultaneous PFAS rejection and photodegradation, with defluorination efficiencies of 60–85% for PFOA under UV-A irradiation. Coupling adsorption-enhanced concentration of PFAS near reactive sites with photocatalysis overcomes the mass-transfer limitation of dilute-phase photocatalysis, where PFAS at ppt concentrations react too slowly with bulk-phase radicals to achieve effective degradation.

Persulfate-based AOPs using heat-, UV-, or metal-activated persulfate to generate sulfate radicals (SO₄•-) show particular promise for PFAS mineralization because sulfate radicals have sufficient oxidation potential ($E^\circ = 2.5\text{--}3.1$ V vs. NHE) and sufficient selectivity to attack terminal CF₃ groups and initiate sequential chain-shortening reactions. Research priorities include developing modified adsorbents that also function as persulfate activators (e.g., iron-doped biochar, manganese oxide-functionalized graphene), enabling single-material simultaneous adsorption and oxidative destruction cycles. The HALT process described in Section 4.3.6 represents a thermally activated variant of this concept and provides proof of concept for the simultaneous adsorption-destruction paradigm^[114].

4.4.2. Electrochemical Treatment Integration

Electrochemical systems play a uniquely versatile role in PFAS remediation, serving simultaneously as: (a) a driving force for concentrating PFAS onto electrode surfaces (electrosorption), (b) a regeneration mechanism for spent adsorbents (electro-regeneration via polarity reversal), and (c) a destruction mechanism for concentrated PFAS in regeneration brines (electrochemical oxidation). Integrating these three functions into a single electrochemical cell offers a transformative opportunity for closed-loop PFAS treatment.

Boron-doped diamond (BDD) electrodes are the most studied electrocatalytic materials for PFAS destruction, achieving >99% PFOA degradation with 84% defluorination at bench scale. However, BDD electrode costs (\$500 – 2000/m²) currently limit full-scale deployment. Research is needed on alternative high-activity electrode materials, including Ti4O7 Magneli phase ceramics, SnO₂-doped materials, and carbon nanotube arrays, which may offer lower production costs. Dimensionally stable anodes (DSA) based on mixed metal oxides (IrO₂-Ta₂O₅) represent a near-term commercial option for electrochemical PFAS treatment in conjunction with adsorptive concentration.

Electrochemical regeneration of conductive adsorbents (activated carbon, graphene-based materials, conductive polymer composites) by applying a reverse potential has been demonstrated at bench scale with promising results (Section 4.3.7). Key research priorities include: scaling electrochemical regeneration to bed-scale packed columns, characterizing performance degradation over >50 electrochemical cycles, understanding the fate of PFAS during electrochemical desorption (are they destroyed in-situ or transferred to the electrolyte?), and developing composite adsorbent-electrode materials that combine high PFAS affinity with sufficient electrical conductivity for effective electrochemical cycling.

4.4.3. Membrane System Integration

Nanofiltration (NF) and reverse osmosis (RO) are effective at rejecting PFAS, achieving over 95% rejection for long-chain PFAS and 80–95% for short-chain PFAS. However, these processes generate concentrated reject streams that require further treatment and are energy-intensive, consuming between 0.5 and 3 kWh/m³. Integrating adsorption pre-treatment with membrane systems can significantly mitigate membrane fouling, extend the service life of membranes, and reduce the volume of high-concentration reject streams that necessitate downstream treatment.

Several adsorption-membrane hybrid configurations have been proposed, including: (a) dosing powdered adsorbents upstream of microfiltration membranes (similar to submerged membrane bioreactor systems), where modified adsorbents pre-adsorb PFAS, allowing the membrane separation to retain the laden particles; (b) adsorbent-coated membranes that combine size exclusion with chemical affinity in a single unit; and (c) adsorption preconcentration followed by RO or NF polishing to ensure ultra-low MCL compliance.

Key research priorities include developing adsorbents that are optimized for stable dispersion in membrane feed streams without causing irreversible fouling, and assessing the trade-off between the costs of adsorption pre-treatment and the frequency of membrane replacement under various PFAS loading conditions.

Membrane distillation (MD) is a thermally-driven membrane process proposed for the concentration and destruction of PFAS within a single unit. PFAS-contaminated brine resulting from adsorption regeneration can be further concentrated using MD, which reduces the volume needing thermal destruction or electrochemical treatment dramatically. Tow et al. (2021) identified MD as a crucial enabling technology for managing membrane concentrate in PFAS treatment trains, although challenges such as PFAS sorption onto hydrophobic MD membranes and pore wetting by fluorosurfactants remain active areas of research.^[115]

4.4.4. AI-Assisted Material Design and Process Optimization

Artificial intelligence and machine learning (ML) approaches are increasingly applied to accelerate PFAS adsorbent discovery and optimize treatment process design, reducing the time and cost of experimental screening across the enormous space of possible modification strategies, PFAS structures, and water matrix conditions.

In material discovery, ML models trained on existing adsorption datasets have been used to predict adsorption capacity across PFAS chain lengths and functional groups for a given adsorbent type. High-throughput computational screening using density functional theory (DFT) and molecular dynamics (MD) simulations, informed by ML-predicted binding energies, can pre-screen thousands of candidate modification chemistries before experimental synthesis. This computational-experimental feedback loop has reduced material development timelines from years to months in analogous applications in pharmaceutical discovery and battery electrode optimization. The primary data challenge for PFAS applications is the relatively small size and inconsistency of existing experimental datasets (varying PFAS structures, water matrices, pH, and competitive ions), which limits ML model generalizability. Concerted data-sharing initiatives and standardized testing protocols would significantly accelerate AI-assisted material discovery.

In process optimization, ML models can predict breakthrough curves in fixed-bed adsorption systems as functions of PFAS influent concentration, flow rate, water quality parameters, and adsorbent properties, enabling real-time adaptive process control that optimizes bed exhaustion timing and regeneration scheduling. Digital twin models of full-scale adsorption systems, calibrated with continuous online PFAS monitoring data, could enable predictive maintenance strategies that reduce both PFAS breakthrough risk and unnecessary early regeneration, thereby minimizing energy and chemical consumption. Several water utilities in North America and Europe are already piloting continuous online PFAS monitoring with immunoassay-based sensors, which could serve as data inputs for AI-driven control systems. Integrating AI-optimized process control with the enhanced materials discussed in this review represents the most direct pathway to cost-effective compliance with the 2024 EPA PFAS MCLs across the diverse water treatment contexts present in the United States and globally.

In regeneration optimization, reinforcement learning approaches can be applied to identify optimal regeneration protocols (solvent composition, temperature, contact time, pH swing sequences) as functions of adsorbent loading state, contaminant profile, and available regeneration resources. This is particularly valuable for multi-contamination scenarios where PFAS co-exist with heavy metals, NOM, or other organic micropollutants, and where simple single-step regeneration protocols leave residual co-contaminants that reduce subsequent PFAS capacity. The stepwise methanol-acid regeneration strategy reported by Chaudhary et al. (2024) for biochar treating PFAS and heavy metal co-contamination illustrates the kind of multi-step sequence that AI optimization could further improve and generalize across adsorbent types^[94].

The convergence of AI-assisted material design, process optimization, and continuous online monitoring, together with the advanced surface-modified adsorbents reviewed here, defines the research frontier for PFAS remediation. Progress in this area requires interdisciplinary collaboration between materials chemists, environmental engineers, data scientists, and regulatory scientists, and will benefit from open-data frameworks that allow ML models to be trained on the full body of published PFAS adsorption research rather than individual laboratory datasets.

Recent advances in AI-driven sustainability assessments and green material fabrication further underscore the transformative potential of these approaches: Pusuluru et al. (2026) demonstrate how AI-driven innovations can optimize biomass utilization and sustainability outcomes in resource recovery systems^[116], while Abbaszadeh et al. (2026) illustrate how AI-integrated manufacturing and green fabrication frameworks are being applied across energy storage, catalysis, and environmental remediation domains, providing methodological templates directly transferable to PFAS adsorbent optimization^[117]. Building on this, Punna et al. (2026) further demonstrate how AI-integrated manufacturing of advanced materials advances energy storage, catalysis, and environmental applications, reinforcing the cross-disciplinary value of AI-driven material design for PFAS remediation^[118]. Singh et al. (2026) further extend this framework by applying machine learning-assisted techno-economic assessment to microalgal biofuel production pathways, offering a rigorous cost-performance evaluation methodology directly applicable to scaling next-generation PFAS adsorbent systems^[119].

4.5. Comparative Analysis of Surface Modification Strategies

The preceding sections have individually described carbon-based, clay-based, chitosan-based, graphene-based, ion-exchange, cyclodextrin, and MOF-based adsorbents. However, selecting the most appropriate strategy for a given application requires a systematic comparison of each class across multiple dimensions: adsorption performance, selectivity toward short-chain versus long-chain PFAS, scalability of production, regeneration efficiency, cost, and practical applicability. Table 4 consolidates these dimensions to support evidence-based adsorbent selection.

Adsorbent class	Key advantages	Key disadvantages	Short-chain PFAS performance	Long-chain PFAS performance	Scalability	Regeneration efficiency	Estimated cost	Practical applicability
Carbon-based (AC, biochar, ACF)	Large surface area; well-established technology; broad PFAS removal	Limited short-chain PFAS selectivity; NOM competition; frequent regeneration needed	Low–moderate (PFBA, PFBS poorly removed by unmodified AC)	High (PFOS, PFOA up to 200 mg/g)	High; commercially mature; granular/powdered forms available	Moderate (solvent/thermal; 85–99% after modification)	Low–moderate (\$0.05–2/kg); centralized thermal reactivation adds cost	Widely deployed in municipal water treatment; best for long-chain-dominated matrices
Clay-based (montmorillonite, diatomite, zeolite)	Abundant and low cost; tunable interlayer spacing; good PFOS/PFOA capacity after organo-modification	Low native surface area; pH-sensitive; challenging post-treatment separation	Moderate after organo-modification (CTAC, IL coatings)	High after organo-modification (up to 151.5 mg/g PFOS; 66.2 mg/g PFOA)	Moderate; raw minerals are abundant, but modification adds steps	High (>98% with methanol/NaCl for IL-modified clay; 5 cycles without loss)	Low (raw clay \$0.01–0.10/kg); modification costs vary by reagent	Promising for point-of-use and developing-world applications due to material abundance
Chitosan-based (MIP, quaternized, crosslinked)	Bio-derived; tunable via crosslinking and grafting; excellent PFOS selectivity via MIP	pH-dependent; limited mechanical strength; acidic degradation	Moderate–high with amino/quaternary ammonium functionalization	High (MIP: up to 560 µmol/g PFOS; quaternized: ~38.7 mg/g PFOS)	Low–moderate; bio-extraction and crosslinking add process steps	High (NaOH/acetone; >98% over 7 cycles for MIP; >98% over 10 cycles for MQCG)	Moderate (\$2–8/kg depending on grade and modification)	Suited for selective PFAS capture in complex matrices; regenerable for multiple cycles
Graphene-based (GO, rGO, PAGO, GO-CTAC)	Extremely high surface area; multi-mechanism binding; near-instant kinetics for cationically modified variants	High production cost; aggregation; difficult scale-up; gradual surfactant loss on regeneration	Very high for cationic modifications (PAGO: 602 mg/g PFBA; GO-CTAC: ~100% removal of 11 PFAS)	Highest reported capacities (PAGO: 2180–3070 mg/g PFOA/PFOS)	Low currently; sheet exfoliation and functionalization remain lab-scale challenges	Moderate (GO-CTAC: 78–95% over 5 cycles; PAGO: closed-loop with PFAS destruction)	High (\$50–200/kg for functionalized GO); cost is the primary barrier	Best suited for high-performance, small-footprint applications; not yet cost-competitive at municipal scale
Ion-exchange resins (single-use, regenerable, quaternary ammonium)	Dual mechanism (ion exchange + hydrophobic); high removal across chain lengths; well-characterized	High material cost; co-ion competition; fouling by NOM; regeneration generates brine waste	High for quaternary ammonium resins (MIEX GOLD: >99% for PFBA, PFBS)	Very high (DR4: 3300 mg/g PFOA; MIEX GOLD: 1.01–1.05 g/g PFHxS/PFOA)	High; commercially available; packed-bed column systems well-established	High (10% NaCl + 30% methanol; 90% over 5 cycles for POP resins)	High (\$5–15/kg); but lifecycle cost can be competitive (\$0.10–0.80/m ³ treated)	Widely applicable in municipal and industrial settings; preferred for strict ppt regulatory compliance

Adsorbent class	Key advantages	Key disadvantages	Short-chain PFAS performance	Long-chain PFAS performance	Scalability	Regeneration efficiency	Estimated cost	Practical applicability
Cyclodextrin-based polymers (β -CD, amine- β -CD)	Host-guest selectivity; strong GenX binding; multi-mechanism (electrostatic + inclusion complex)	High cost for pure CDs; limited cavity size for longer PFAS; lower capacity vs some conventional sorbents	High for short-chain PFAS including GenX; amine- β -CD shows 100 $\times$ higher affinity for PFOA vs GenX	Good for medium-chain PFAS; less competitive vs AC/resin for very long chains	Low-moderate; polymer cross-linking adds production complexity	Good (methanol/water 70:30; 89% capacity retained after 6 cycles)	High (\$10-30/kg); cost decreases with polymer network approaches vs pure CD	Niche application for short-chain and branched PFAS that evade conventional adsorbents
MOF-based (functionalized, water-stable)	Tunable pore geometry; adjustable fluorophilic/electrostatic ligands; strong short-chain PFAS binding	High synthesis cost; aqueous instability of many MOFs; limited pilot-scale data; metal leaching risk	High for water-stable MOFs with fluorophilic ligands (up to 86% short-chain removal; bio-MOF: 80-100%)	High for long-chain PFAS (MOF PSM variant: 783 mg/g PFOA)	Very low currently; complex ligand synthesis and aqueous stability remain barriers	Moderate (solvent regeneration; reusability demonstrated but long-term cycling limited)	Very high (\$100-500/kg); cost is the primary obstacle to deployment	Research-stage for most variants; most promising for ultra-trace short-chain PFAS removal where conventional adsorbents fail

Table 4. Comparative Analysis of Surface-Modified Adsorbent Classes for PFAS Removal

Several cross-cutting observations arise from this comparison. First, for long-chain PFAS (such as PFOS, PFOA, and PFDA), carbon-based and ion-exchange resin systems currently provide the best balance of high capacity, scalability, and cost-effectiveness, rendering them the leading technologies for municipal-scale treatment. **Second**, when it comes to short-chain PFAS (including PFBS, PFBA, GenX, and PFHxS), cationic modifications, particularly quaternary ammonium-functionalized materials, amine-crosslinked cyclodextrin polymers, and fluorophilic metal-organic frameworks (MOFs), exceed the performance of hydrophobic-only adsorbents. This is due to electrostatic and fluorous interactions that effectively compensate for the lower hydrophobicity of shorter fluorocarbon chains. Third, while graphene-based materials exhibit the highest absolute adsorption capacities documented in the literature, their cost and scalability limitations confine their application to specialized contexts. Fourth, clay-based and chitosan-based materials present the most favorable sustainability profile, given their bio-derived or earth-abundant precursors, which is particularly significant for decentralized or low-resource environments. Finally, regeneration efficiency is most robust for covalently grafted modifications (such as quaternized chitosan, ATRP-grafted polymers, and molecularly imprinted polymers, MIPs), whereas physically adsorbed surfactant coatings (like organo-clays and certain GO-CTAC materials) tend to lose 10-20% of their capacity over five cycles due to surfactant desorption during the regeneration process. These distinctions should inform the selection of adsorbents for specific deployment contexts and direct future research priorities for next-generation materials.

4.6. Comparative Ranking of Best-Performing Adsorbents for PFAS Removal

To provide a concise practical reference, Table 5 ranks the best-performing adsorbents reported in the literature separately for short-chain PFAS (carbon chain length C4-C6) and long-chain PFAS (C8 and above), based on maximum reported adsorption capacity (mg/g), removal efficiency under environmentally relevant conditions, and reproducibility across the reviewed studies. This ranking is intended to assist practitioners and researchers in identifying priority candidate materials for specific treatment objectives.

Rank	Adsorbent	Modification	Target PFAS	Best reported capacity (mg/g or removal %)	Primary mechanism(s)	Reference(s)
1	Polyamine-layered graphene oxide (PAGO)	1-nm polyamine adlayer on GO nanosheets	PFBA (C4), PFPrA (C3)	602 mg/g (PFBA); 220 mg/g (PFPrA); ~100% removal in minutes	Electrostatic attraction, H-bonding, F-F interactions	[57]
2	Porous aromatic framework (PAF) with fluorous + electrostatic segments	Combined quaternized and fluorinated functional segments	PFBA, PFBS, GenX	24.1× improvement over GAC for PFOA; best single mechanism for short-chain PFAS	Fluorous interactions dominant; electrostatic supplementary	[72]
3	Ion-exchange resin DR4 (crosslinked DADMAC/BisAAM beads)	Quaternary ammonium polymer beads with enhanced porosity	PFBA, PFBS, PFHxS, GenX	3300 mg/g (PFOA); >99.9% removal at 50 BV for all tested PFAS	Electrostatic (ion exchange), hydrophobic, H-bonding	[120]
4	GO modified with CTAC (GO-CTAC)	Cetyltrimethylammonium chloride surfactant grafting on GO	11 PFAS including short-chain (GenX, PFBS)	~100% removal of all 11 PFAS in 1 h	Electrostatic attraction, hydrophobic interactions	[121]
5	Amine-crosslinked β -cyclodextrin polymer	Tripodal amino crosslinker with β -CD cavities	GenX, PFOA, short-chain PFAS	100× higher affinity for PFOA vs GenX; strong GenX binding vs amido variant	Host-guest inclusion + electrostatic interactions	[65]
6	Quaternary ammonium-grafted flax fibers (ATRP)	Poly(METAC) grafting via surface-initiated ATRP	PFBA, PFBS (C4–C6)	>78% PFBS and >97% PFBA removal (1 cycle)	Electrostatic (quaternary ammonium anion exchange)	[66]
7	Water-stable bio-MOF CuI2(S,S)-hismox	Bio-derived Cu-MOF with fluorophilic binding sites	Short-chain PFAS (C4–C6)	Up to 86% short-chain PFAS removal with rapid kinetics	Electrostatic, H-bonding, fluorophilic interactions	[62]

Table 5a. Best-Performing Adsorbents for Short-Chain PFAS Removal (C4–C6, including GenX)

Rank	Adsorbent	Modification	Target PFAS	Best reported capacity (mg/g)	Primary mechanism(s)	Reference(s)
1	Polyamine-layered graphene oxide (PAGO)	1-nm polyamine adlayer on GO nanosheets	PFOS, PFOA	2180–3070 mg/g (PFOA/PFOS)	Electrostatic attraction, hydrophobic, H-bonding, F-F interactions	[52]
2	Ion-exchange resin DR4 (crosslinked DADMAC/BisAAm beads)	Quaternary ammonium polymer beads	PFOA, PFOS, PFHxS	3300 mg/g (PFOA)	Electrostatic (ion exchange), hydrophobic, H-bonding	[120]
3	Molecularly imprinted polymer (PFOS template, chitosan matrix)	Electropolymerized o-PD with PFOS template	PFOS, PFHxS	Up to 1455 mg/g (PFOS)	Selective cavity recognition, electrostatic, hydrophobic	[47][122]
4	Functionalized MOF (post-synthetic modification)	Post-synthetic modification (PSM) of MOF scaffold	PFOA	783 mg/g (PFOA)	Lewis acid-base interactions, electrostatic, pore filling	[123]
5	IL-modified montmorillonite clay	Imidazolium ionic liquid modification	PFOS, PFOA	151.5 mg/g (PFOS); 66.2 mg/g (PFOA)	Hydrophobic, electrostatic, interlayer expansion	[124]
6	Red mud-modified sawdust biochar (RMSDN600)	Red mud mineral oxide impregnation	PFOS	194.6 mg/g (PFOS at pH 3.1)	Hydrophobic interactions, protonated metal groups	[125]
7	Few-layered porous graphite (EPG)	Physical exfoliation of graphite layers	PFOS	Multilayer high capacity (intercalation model)	Electrostatic+hydrophobic (intercalation)	[126]
8	KOH-activated spent coffee ground biochar (SCGKOH)	KOH chemical activation of biochar	PFOS	43.4 mg/g (PFOS); 99.6% removal	Hydrophobic interaction via C-F chain	[127]
9	Quaternized cotton (ATRP polymer brushes)	Quaternary ammonium polymer brushes via ATRP	PFOS, PFOA	3.3 mmol/g (PFOS); 3.1 mmol/g (PFOA) at pH 5	Anion exchange (electrostatic)	[9]
10	Activated carbon fibers (PACF, polyacrylonitrile-based)	Thermal activation of PAN-based fibers	PFOS, PFOA	Higher capacity than commercial GAC (multiple orders of magnitude in some conditions)	Hydrophobic + electrostatic (multilayer/micelle)	[128]

Table 5b. Best-Performing Adsorbents for Long-Chain PFAS Removal (C8+, including PFOS and PFOA)

Notes: The capacities noted are the maximum values reported under optimal laboratory conditions (such as single-compound scenarios, synthetic water, and optimized pH levels). In real-world applications involving complex matrices with natural organic matter (NOM), competing ions, and mixed per- and polyfluoroalkyl substances (PFAS), actual performance is likely to be lower. The rankings take into account a combination of reported maximum capacities, the range of PFAS types addressed, and the reproducibility of results across independent studies. In cases where capacity data was not directly comparable (for instance, when reported solely as removal percentages), the ranking was based on removal efficiency at environmentally relevant initial concentrations.

5. Environmental Implications of Adsorbent Disposal

While adsorption effectively removes PFAS from water, managing PFAS-laden adsorbents poses significant environmental challenges. Improper disposal can result in secondary pollution risks due to leaching or the thermal release of PFAS compounds. Therefore, it is crucial to adopt safe end-of-life management strategies. Potential solutions include high-temperature incineration, advanced oxidation techniques to degrade PFAS before disposal, and integrating adsorbents into circular-economy frameworks, allowing for regeneration or repurposing. Future research should prioritize life-cycle assessments that not only evaluate adsorption efficiency but also consider the environmental impact associated with the disposal of adsorbents.

Sustainable end-of-life management strategies can draw inspiration from plastic waste valorization methods, such as converting PET into carbon-based nanomaterials for environmental remediation. This approach demonstrates how waste streams can be transformed into functional adsorbents, thereby minimizing the risk of secondary pollution^[129].

6. PFAS in Emerging Pollutant Frameworks

PFAS contamination should be understood within the wider context of emerging pollutant management frameworks. Recent studies emphasize the significance of integrated treatment approaches that concurrently address multiple classes of contaminants, such as pharmaceuticals, pesticides, and microplastics. Adsorbents designed for PFAS removal may also interact with co-contaminants, presenting both opportunities and challenges for multi-pollutant remediation efforts. By situating PFAS research within these frameworks, we can ensure that treatment technologies remain pertinent to evolving environmental priorities.

Furthermore, it is crucial to consider the broader pathways of contamination. For example, groundwater contamination by microorganisms illustrates how various classes of pollutants interact within aquifers, highlighting the importance of risk assessment frameworks that incorporate PFAS migration alongside both biological and chemical contaminants^{[130][131]}.

7. Groundwater Contamination Pathways and Risk Assessment

PFAS contamination in groundwater is influenced by the unique physicochemical properties of individual congeners. Long-chain PFAS compounds, such as PFOS and PFOA, tend to create persistent and expansive subsurface plumes that originate from point sources like AFFF application sites, landfill leachate infiltration zones, and industrial discharge areas. In contrast, short-chain congeners have lower soil-water partition coefficients, resulting in enhanced mobility in the subsurface and making them significantly more challenging to intercept and remediate^[4]. The amphiphilic nature of PFAS leads to their preferential accumulation at soil-water and air-water interfaces in the vadose zone. This phenomenon creates a secondary source of contamination that can be remobilized during rainfall infiltration events and fluctuations in the water table. Additionally, hydrogeological heterogeneity, such as preferential flow through fractures and high-conductivity lenses, can facilitate the delivery of PFAS pulses to the saturated zone at rates significantly surpassing those predicted by homogeneous transport models^[4]. Exposure to PFAS-contaminated groundwater occurs via several pathways that collectively influence the total human and ecological dose. The primary route is the direct ingestion of contaminated drinking water from private wells and community supplies. Chronic low-level exposure has been associated with various health issues, including thyroid dysfunction, immunosuppression, dyslipidemia, and an increased risk of cancer^[11]. Secondary pathways, such as bioaccumulation through aquatic food webs fed by PFAS-impacted groundwater baseflow, crop uptake from agricultural irrigation, and dermal contact during recreational activities, further elevate the total body burden beyond what water ingestion alone would suggest^[132]. Risk assessment frameworks have evolved from single-compound deterministic approaches to cumulative mixture models that more accurately represent the multi-congener co-occurrence commonly found at real contaminated sites. Regulatory frameworks, such as the US EPA's National Primary Drinking Water Regulation, have formalized hazard index approaches for PFAS mixtures in drinking water^[15]. These considerations have significant implications for the adsorbent-based remediation technologies discussed in this paper. Risk-derived remediation endpoints, such as maximum contaminant levels or ecological screening values, directly influence the required quality of effluent, the selection of adsorbents, the design of bed volumes, and the frequency of regeneration. Additionally, the presence of natural organic matter, competing co-contaminants, and complex multi-congener PFAS mixtures in contaminated groundwater poses performance challenges that must be addressed to ensure that laboratory-scale adsorption results are effectively translated into field-scale risk reduction^{[33][70]}.

8. Conclusion

This review synthesizes current advancements in surface-modified adsorbents for the removal of PFAS, emphasizing material design strategies, adsorption mechanisms, and regeneration approaches. Although notable progress has been achieved, several knowledge gaps and unresolved challenges remain. These include inconsistent performance with short-chain PFAS, limited validation under real-world water matrices, and uncertainties regarding long-term stability and the feasibility of regeneration. Addressing these gaps will necessitate standardized testing protocols and comparative studies to reconcile conflicting findings.

Beyond laboratory-scale performance, the environmental implications of adsorbent disposal must be carefully considered. PFAS-laden adsorbents present risks of secondary pollution if not managed appropriately, highlighting the importance of safe end-of-life strategies, such as advanced oxidation, incineration, or conversion into functional carbon-based materials. It is equally crucial to embed PFAS remediation within emerging pollutant management frameworks, as contamination often occurs alongside pharmaceuticals, pesticides, and microorganisms in groundwater systems. Developing risk assessment models that integrate PFAS migration with broader contaminant pathways will enhance the environmental relevance of remediation technologies.

Looking ahead, artificial intelligence and machine learning present transformative opportunities for adsorbent design, performance prediction, and process optimization. AI-driven frameworks can accelerate material discovery, optimize regeneration cycles, and improve techno-economic feasibility, bridging the

gap between laboratory innovations and industrial deployment. Concurrently, sustainability considerations including resource consumption, circular economy principles, and life-cycle environmental footprints must guide future research to ensure that remediation strategies are both effective and responsible.

Ultimately, the future of PFAS remediation lies in integrated treatment systems that combine adsorption with destructive technologies such as advanced oxidation, electrochemical processes, and membrane filtration. When paired with AI-assisted optimization and sustainability assessments, these hybrid approaches can offer scalable, cost-effective, and environmentally sound solutions. By contextualizing PFAS research within broader frameworks of emerging contaminants, sustainable remediation, and data-driven innovation, this review underscores the necessity for interdisciplinary collaboration to achieve long-term protection of water resources and public health.

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During the preparation of this work, the author(s) used Grammarly and Claude.ai to improve the manuscript. After using this tool/service, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the published article.

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