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The PFAS nexus: a critical review linking toxicity, remediation, and emerging artificial intelligence applications

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ABSTRACT

Per- and polyfluoroalkyl substances (PFAS) comprise a structurally heterogeneous class whose reported size varies with the operational definition and inventory used. Their environmental persistence, mobility, and widespread occurrence have created substantial challenges for exposure assessment, toxicological characterization, and remediation. This review critically integrates three connected domains: molecular and systems toxicology, destructive and non-destructive remediation technologies, and emerging artificial intelligence and machine-learning (AI/ML) applications. The toxicology section emphasizes the strength of evidence across metabolic, endocrine, hepatic, immune, reproductive, epigenetic, and carcinogenic outcomes, while avoiding extrapolation from a small number of well-studied legacy compounds to the full PFAS chemical space. Remediation approaches are compared by contaminant range, treatment outcome, evidence for defluorination or mineralization, relative energy demand, residual generation, and major implementation limitations, with expanded coverage of non-thermal plasma, fungal biotransformation, microbial consortia, and hybrid physicochemical-biological treatment. For AI/ML, we distinguish PFAS-specific demonstrations from methods transferred from adjacent fields and from longer-term research concepts that remain unvalidated. We define the PFAS Nexus as a conceptual decision framework that links hazard evidence, treatment selection, data quality, and regulatory needs rather than as a validated predictive model. The synthesis identifies priority needs for transparent datasets, external model validation, mass-balance and fluoride-recovery measurements, matrix-realistic biological studies, and pilot-scale evaluation of integrated treatment trains.

1. Introduction

Per- and polyfluoroalkyl substances (PFAS) are a diverse group of fluorinated chemicals used in industrial processes and consumer products because fluorinated carbon frameworks can confer thermal stability, chemical resistance, and surface-active properties (Gaines, 2023). These same properties contribute to persistence and complicate degradation, particularly for highly fluorinated terminal perfluoroalkyl acids. PFAS occurrence has been documented in surface water, groundwater, precipitation, wildlife, and human biomonitoring samples, although concentrations and exposure pathways vary substantially among regions and source types (Zhang et al., 2025; Zheng et al., 2023). Under the OECD structural definition, the PFAS universe can include fluorinated surfactants, polymers, intermediates, pharmaceuticals, pesticides, and other xenobiotics containing qualifying fluorinated carbon motifs; therefore, not every fluorinated compound has the same environmental

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behavior, exposure profile, or toxicological evidence base (Wang, 2021). Although the C-F bond remains highly resistant to biodegradation, recent studies have reported partial defluorination of selected precursors, compound-specific transformations, and microbial or enzymatic degradation of ether-containing and unsaturated PFAS; however, these findings have not achieved broad or complete mineralization of terminal PFAA (Yu et al., 2022; Jin et al., 2025).

The reported number of PFAS is inventory-dependent rather than a single fixed value. The 2023 REACH restriction dossier prepared by authorities from Denmark, Germany, the Netherlands, Norway, and Sweden estimated that approximately 10,000 PFAS fall within its regulatory scope, whereas the US EPA CompTox PFASSTRUCTV6 list contains 21,028 records with explicit structures under its operational structural filters (European Chemicals Agency, 2023). These values should not be treated as contradictory because the lists differ in purpose, inclusion criteria, treatment of polymers and mixtures, and database curation. Commercial uses include aqueous film-forming foams, fluoropolymer production, semiconductor processing, textiles, coatings, food-contact materials, and selected pharmaceutical and agrochemical applications (Gaines, 2023). Evidence from epidemiological, experimental, and mechanistic studies links selected PFAS, especially PFOA and PFOS, with perturbations in lipid metabolism, liver function, immune responses, thyroid signaling, reproduction and development, and carcinogenicity (International Agency for Research on Cancer (IARC) 2025, Rappazzo et al., 2017; Shirke et al., 2026). However, the evidence is highly uneven across substances, endpoints, species, doses, and exposure durations. Most PFAS have little or no directly interpretable toxicological information, and estimates of the characterized fraction depend on both the chemical inventory and the minimum evidence threshold. Limited substance-specific evidence is therefore a central data-coverage problem for hazard assessment.

Recent case studies highlight substantial variation in PFAS composition, concentration, analytical sensitivity, and associated human and ecological Perfluoropentanoic relevance across environmental matrices and geographical regions. Table 1 provides a comparative summary of these studies by PFAS type detected, concentration range, analytical method, and associated health or environmental risks. Thus, it highlights the heterogeneity of PFAS occurrence and the need for integrated assessment approaches.

This review goes beyond a conventional descriptive overview by critically integrating three linked domains: mechanistic toxicology, remediation performance, and emerging AI/ML applications. Specifically, we evaluate which toxicity mechanisms are sufficiently supported to guide hazard prioritization; which remediation technologies achieve removal, transformation, partial defluorination, or mineralization under environmentally relevant conditions; and where AI/ML has generated PFAS-specific evidence, versus where its role remains transferable or prospective. The PFAS Nexus is defined here as a conceptual evidence-to-decision framework connecting chemical identity and exposure, mechanistic hazard data, treatment performance and byproducts, data quality, and regulatory or implementation constraints. This integrated perspective distinguishes the present review from studies that address these domains independently and is intended to identify evidence gaps rather than imply the existence of a universally validated prediction or treatment platform.

Several recent reviews have addressed PFAS use patterns (Gaines, 2023), contamination, exposure, and health risks in developing countries (Anik et al., 2025), PFAS analytical determination methods (Idowu et al., 2025), toxicological evidence from a cheminformatics perspective (Papathanasiou et al., 2026), and PFAS-contaminated wastewater remediation technologies (Farina et al., 2026). However, these domains have largely been evaluated independently with limited translation between hazard evidence, environmental occurrence, treatment selection, and emerging computational tools. The distinctive aim of the present review is therefore not to provide another descriptive inventory of PFAS studies, but to integrate mechanistic toxicology, treatment performance, biological and physicochemical remediation, and AI/ML within an evidence-calibrated decision framework. We distinguish parent-compound removal from transformation, partial defluorination, and mineralization; evaluate emerging treatment approaches in terms of matrix dependence, residual generation, energy demand, and technology readiness; and classify AI/ML applications as PFAS-specific demonstrations, transferable methodologies, or prospective concepts. This integrated approach identifies where evidence streams converge, where important decision gaps remain, and which research directions require additional validation before regulatory or field implementation.

2. PFAS: environmental fate and transport, regulatory guidelines, and literature gap

2.1. Environmental fate, transport, and planetary-scale contamination

PFAS enter the environment through manufacturing and processing discharges, use of aqueous film-forming foams at military and civilian facilities, landfill leachate, wastewater and biosolids, and transformation of volatile or semi-volatile precursors (Conder et al., 2008). Cousins et al. reported that measured PFOA concentrations in rainwater commonly exceeded the US EPA 2022 interim lifetime health advisory of 0.004 ng L^{-1} (Cousins et al., 2022; U.S. Environmental Protection Agency, 2022). That advisory was a non-enforceable, health-based benchmark and should not be confused with the enforceable 4 ng L^{-1} maximum contaminant level (MCL) established for PFOA in the 2024 drinking-water regulation.

Across different environmental and exposure matrices, PFAS contamination has been documented, showing that contamination extends beyond localized industrial sites. For example, in the U.S., PFAS in public drinking water has been statistically associated with industrial facilities, wastewater treatment plants, military fire-training areas, and aqueous film-forming foam (AFFF)-related sources (Hu et al., 2016). Frequent PFAS detection was observed in shallow groundwater in Wisconsin, with at least one PFAS detected in 71% of samples (Silver et al., 2023). Broader groundwater surveys confirm the detection of 14 out of 24 PFAS, with higher detection frequency in public wells than in domestic wells, highlighting the influence of hydrogeology and surrounding land use (McMahon et al., 2022). PFAS detection is also evident in indoor and wastewater-related environments. For example, ultra-short- and short-chain PFAAs (e.g., TFA and PFPrA) are frequently reported in residential environments, mainly due to contributions from atmospheric, waterborne, indoor, and consumer-product sources (Zheng et al., 2023). Municipal and industrial inputs during domestic or industrial wastewater treatment are a major pathway for PFAS release (Desgens-Martin et al., 2023).

Persistent groundwater PFAS contamination is observed at AFFF-impacted military fire-training sites (Ruyle et al., 2023). Sea-spray aerosols can facilitate PFAS spread through ocean-to-atmosphere re-emission of perfluoroalkyl acids (Johansson et al., 2019), and their long-range transport and environmental recirculation lead to PFAS detection in rainwater and drinking water (Cousins et al., 2022). Long-range atmospheric transport of volatile and semi-volatile PFAS precursors, followed by atmospheric transformation and deposition, contributes to PFAS occurrence in remote regions, including Arctic and Antarctic environments (Kwok et al., 2013; Harb et al., 2026). Enrichment within the ocean surface microlayer further promotes marine aerosol emissions and bidirectional atmosphere-ocean exchange, thereby creating a self-reinforcing global transport cycle (Johansson et al., 2019). Biomagnification of PFCAs within aquatic food webs is strongly chain length-dependent; PFCAs containing 10–14 carbons exhibit biomagnification factors ranging from 3 to 15 in Arctic marine mammal food chains (Boisvert et al., 2019). Consequently, PFCA concentrations in polar bear liver may range from ng g^{-1} to μg g^{-1}, highlighting substantial long-term exposure risks (Fig. 1) (Conder et al., 2008).

Table 1
Representative case studies of PFAS contamination in different environmental matrices, major PFAS, analytical coverage, and associated human-health and environmental relevance.

Geographic location/matrix	Major PFAS	Reported contamination	Analytical method/ detection limit	Human-health risk/ relevance	Environmental risk/ relevance	Reference
PFAS survey from 22 developing countries Sample collection period from 2017 to 2019 Total 144 surface water samples (Africa, n=44; Asia-Pacific, n=60; and Latin America and Caribbean countries, n=40)	Major per- and polyfluoroalkyl substances (PFAS) include: perfluorooctane sulfonic acid (PFOS), perfluorooctanoic acid (PFOA), and perfluorohexane sulfonic acid (PFHxS)	PFOS: 0.03–6.23 ng L^{-1} PFOA: 0.05–4.02 ng L^{-1} PFHxS: 0.03–3.51 ng L^{-1}	Solid phase extraction (SPE), Ultra-performance liquid chromatography coupled with tandem mass spectrometry (UPLC-MS/MS) Limits of quantification (LOQs) of 0.025 ng L^{-1} for linear PFOS, branched PFOS, and PFHxS. The LOQ was 0.05 ng L^{-1} for PFOA	No formal risk estimate reported The study was designed for environmental monitoring	PFOS, PFOA, and PFHxS were quantified in 89%, 85%, and 71% of samples, respectively, establishing a United Nations Environment Programme/Global Monitoring Plan (UNEP/GMP) baseline for trend monitoring PFAS levels varied mainly with sampling location/source Country income and population density were not significant predictors	(Baabish et al., 2021)
PFAS concentration in the Ganges River basin, and groundwater in India	Detected multiple PFAS in the river, particularly short-chain PFAS, such as Perfluorobutane sulfonic acid (PFBS) and PFHxA	Surface water shows PFBS up to 10.2 ng L^{-1} and PFHxA, 0.4–4.7 ng L^{-1} Groundwater shows PFHxA and PFHpA of 0.8 to 4.9 ng L^{-1} and 0.5 to 5.3 ng L^{-1}	Oasis HLB solid-phase extraction (SPE) followed by HPLC-ESI-MS/MS Compound-specific minimum quantification limits (MQLs) ranged from 0.004–8.974 ng L^{-1} (PFBA), 0.46–3.46 ng L^{-1} (PFHxA), 0.017–2.152 ng L^{-1} (PFHpA), and 0.040–51.23 ng L^{-1} (PFBS)	Drinking-water exposure was quantitatively assessed PFHxA intake was highest (up to 0.2 ng kg^{-1} day^{-1}), and children had the highest intake per body weight - Hazard Index (HI) values were <1 for all PFAS and age groups, indicating no considerable oral non-cancer risk under the study assumptions.	The predominance of short-chain PFAS indicated substitution of legacy PFAS. River and groundwater profiles suggested wastewater-affected river water, leakage/ leaching, and/or irrigation-related infiltration as sources of aquifer contamination.	(Sharma et al., 2016)
Distribution of PFASs in surface and bottom water Shuangtaizi Estuary, China	Detected 15 perfluorobutanoic acid (PFBA), perfluoropentanoic acid (PFPeA), PFOA, PFHxA, PFBS, and other PFAS	Observed total concentration of PFAS in surface and bottom water ranged from 66.2–185 ng L^{-1} and 44.8 to 209 ng L^{-1}, respectively.	WAX-SPE-HPLC-ESI-MS/MS Limits of detection (LODs), 0.006 to 0.403 ng L^{-1} and limits of quantifications (LOQs) of 0.021 to 1.342 ng L^{-1}	No case-specific human-health risk assessment was performed Health relevance was discussed from known persistence, bioaccumulation, and toxicity of selected PFAS	High occurrence of mobile short-chain PFAS indicates contamination and transport within the estuarine environment. The estimated flux of 15 PFAS from the Shuangtaizi River to Liaodong Bay was 352 kg $year^{-1}$	(Shao et al., 2016)
Investigated 15 perfluoroalkyl acids (PFAAs) in surface water and sediments of the coastal area in Bangladesh	Detected PFAAs, including C4-14-perfluoroalkyl carboxylates (PFCAs) and C4, C6, C8 and C10-perfluoroalkyl sulfonates (PFSAs) PFOA dominant in water and PFOS in sediment	Estimated ΣPFAAs 10.6–46.8 ng L^{-1} and PFOA 3.17–27.8 ng L^{-1} in surface water Sediment contained ΣPFAAs of 1.07–8.15 ng g^{-1} dry weight (dw) and PFOS 0.60–1.14 ng g^{-1} dw	HPLC–MS/MS LOQs of PFAAs ranged from 0.016 ng L^{-1} in water and 0.006 to 0.102 ng L^{-1} in dry weight of sediment	Potential exposure of PFAAs in the local population through ingestion of fish and shellfish (e.g., Hilsa, Pomfret, Shrimp, and Crab) grown in contaminated water - Quantitative risk NR	Preliminary ecological assessment found hazard quotient (HQ) <1 for PFOA/PFOS for acute pelagic, benthic, and benthopelagic effects. 93% of surface-water samples exceeded the EC PFOS saltwater EQS (0.21 ng L^{-1}), indicating potential long-term risk to pelagic organisms despite low acute risk	(Habibullah-Al-Mamun et al., 2016)
Investigated PFAAs in air and surface water in Dhaka, Bangladesh	Detected ionic PFAS including PFBA, PFHxA, PFOA, PFHxS, and PFOS Neutral PFAS, especially fluorotelomer alcohols (FTOHs, e.g., 6:2 FTOH)	Reported ionic PFAS concentration range of 1.8–19.0 ng L^{-1} in surface water Neutral 6:2 FTOHs were found at 70 ng m^{-3} in air and 1.3 to 11 ng L^{-1} in water	Neutral PFAS detected using GC-MS Ionic PFAS analyzed by WAX-SPE + LC-MS/MS MDLs for major ionic PFAS: PFBA 0.53, PFHxA 0.28, PFOA 0.32, PFHxS 0.05, and PFOS 0.02 ng L^{-1}. 6:2 FTOH passive-sampler	Identified air and water as potential exposure media and noted that textile-related PFAS emissions could be relevant to human and ecosystem health Formal quantitative risk NR	High 6:2 FTOH and short-chain PFAS abundance indicated probable textile-industry sources and a shift toward short-chain alternatives. Industrial effluent from Dhaka may contribute PFAAs to downstream waters	(Morales-McDevitt et al., 2022)

(*continued on next page*)

Table 1 (*continued*)

Geographic location/matrix	Major PFAS	Reported contamination	Analytical method/ detection limit	Human-health risk/ relevance	Environmental risk/ relevance	Reference
			MDL/IDL of 0.25 ng g^{-1} PE		and emphasized precursor transformation, sediment sampling, and nontarget screening.	
Investigated PFAS and alternatives in residential soils in China	Legacy and emerging PFAS, including perfluoro (2-(6-chlorohexyl)oxy) ethanesulfonic acid (6:2 Cl-PFESA)	Reported concentration of 21 PFAS in the range of 244–13,564 pg g^{-1} Among them, PFOA was the dominant compound with a concentration of 354±439 pg g^{-1}	HPLC-triple-quadrupole MS (negative ESI, MRM) LOD and LOQ were considered as 3 and 10 times the signal-to-noise (S/N), respectively	Residential-soil contamination was identified as a potential exposure source through ingestion, inhalation, and dermal contact. Formal risk NR	Short-chain analogs and F-53B were more prevalent than PFOS, demonstrating extensive replacement of legacy PFAS. Residential soil can redistribute PFAS to surface water, groundwater, atmosphere, plants, and the food chain.	(Li et al., 2020)
Former military airfield F18, Stockholm, Sweden Investigated PFAAs from aqueous film-forming foams (AFFF)-impacted soil or long-term contaminated site	Studied PFHxA, PFOA, PFHxS, PFOS in soil, groundwater, surface water, tap water, water well, and fish muscle	Groundwater: ΣPFAAs 738–51,000 ng L^{-1} Surface water: <MDL–79.0 ng L^{-1} PFOS/PFOA persisted in soil >30 years after historical AFFF use The contaminated aquifer supplied ~7,500 m^3 d^{-1} for drinking-water production	WAX SPE HPLC-ESI-MS/MS Calculated method detection limit (MDL) as 3 times the standard deviation of the blank sample and in the range of tens to hundreds of pg per L (water) and per g (solid)	Persistent source may contribute to groundwater and subsequent human exposure. Quantitative risk NR	AFFF-derived PFOS/ PFOA remained in soil >30 years and leached to groundwater and surface waters. Very high PFOS in groundwater and fish demonstrated long-term source persistence, transport, and bioaccumulation around the abandoned airfield.	(Filipovic et al., 2015)

PFAS regulation has gradually moved from individual-substance controls toward broader class- and mixture-oriented approaches. The Stockholm Convention listed PFOS under Annex B in 2009, PFOA under Annex A in 2019, and PFHxS under Annex A in 2022. In April 2024, the US EPA finalized enforceable MCLs of 4 ng L^{-1} for PFOA and PFOS, 10 ng L^{-1} for PFHxS, PFNA, and HFPO-DA, and a hazard-index MCL for mixtures involving these compounds and PFBS (U.S. Environmental Protection Agency, 2024). In May 2026, EPA proposed retaining the PFOA and PFOS MCLs while allowing eligible systems additional compliance time, and separately proposed rescinding the other individual and mixture provisions; these proposals were under public review at the time of revision and should not be described as finalized changes (U.S. Environmental Protection Agency, 2026). In Europe, the national authorities of Denmark, Germany, the Netherlands, Norway, and Sweden prepared and submitted the universal restriction dossier to ECHA in January 2023; ECHA is the receiving and evaluating body, not the author of the proposal (European Chemicals Agency, 2023). In most cases, regulatory ambition outstrips current capacity for treatment and monitoring. Compliance costs depend on PFAS concentration in the source water, the chosen treatment method, residual management, facility size, and implementation time. Rather than assuming that AI/ML will automatically minimize these costs, this review evaluates where data-driven methods may support process optimization and where pilot-scale, PFAS-specific validation remains absent.

2.2. Critical knowledge gaps and review scope

Three critical evidence gaps define the scope of this review: (i) substance-specific hazard evidence covers only a small and structurally unrepresentative subset of the PFAS inventory; (ii) most remediation studies report parent-compound removal but lack fluorine mass balance, transformation-product identification, and field-scale cost assessment; and (iii) many assertions of potential with AI/ML methods are derived from studies on chemicals, materials, or water treatment generally rather than on PFASs specifically. The following sections therefore emphasize evidence quality, applicability domain, and technology readiness rather than novelty claims alone. The dedicated biological remediation and outlook sections critically evaluate recent advances and limitations in microbial, fungal, enzymatic, biofilm-based, and consortium-assisted PFAS transformation.

3. Mechanisms of PFAS toxicity: from molecular targets to system-level disruption

PFAS toxicity occurs via molecular mechanisms that vary in importance depending on chain length, functional group, dose, organism, life stage, and exposure duration (Fig. 2). This section focuses on the most well-established mechanisms, separating mechanistic possibilities from causation in humans. Since mechanistic information remains largely limited to a subset of well-studied legacy PFAS, conclusions should not be generalized across all PFAS structures.

3.1. PPAR pathway dysregulation

PFOA, PFOS, and other PFAS are known to affect peroxisome proliferator-activated receptor (PPAR) pathways and influence transcription programs associated with fatty acid oxidation, lipid metabolism, and inflammatory processes (Vanden Heuvel et al., 2006; Rosen et al., 2010). Receptor activation depends on both a compound's chemical structure and the species under consideration, and rodent responses to PPARα activators cannot be extrapolated to humans. Observational studies in humans, however, report associations between PFAS concentrations and lipid and liver-function biomarkers without demonstrating involvement of the PPAR pathway alone (Nian et al., 2019; Gallo et al., 2012). Experimental data most convincingly show modulation of PPARγ and adipogenic properties, whereas epidemiological research is inconsistent and potentially confounded by co-exposures, diet, and metabolism. Interpretation of PPAR-associated

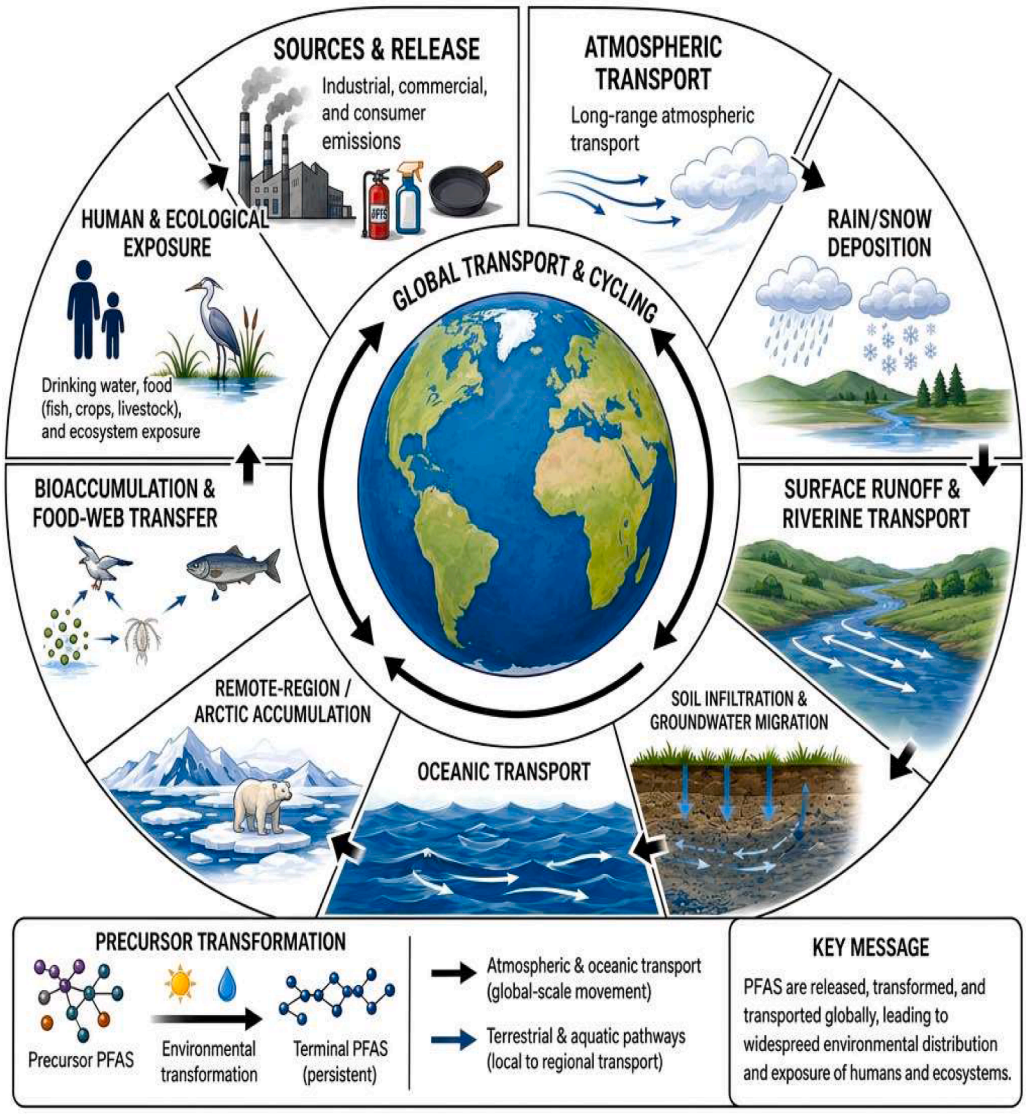

Fig. 1. Source-to-receptor framework for PFAS environmental transport and exposure. Major industrial and consumer-related emission sources are linked to atmospheric transport and deposition, surface-water runoff, soil infiltration, groundwater migration, precursor transformation, aquatic transport, and food-web transfer. The framework illustrates how compound-specific physicochemical properties and environmental matrices govern PFAS mobility, persistence, bioaccumulation, and eventual human and ecological exposure.Regulatory landscape: Stockholm Convention, REACH, and U.S. drinking-water standards.

data should therefore focus on receptor activation by a particular PFAS in a particular species, combined with metabolic evidence, rather than on a single transcriptomic signature (Table 2) (Vanden Heuvel et al., 2006; Rosen et al., 2010; Nian et al., 2019).

3.2. *Thyroid endocrine axis disruption*

PFAS influence the hypothalamic-pituitary-thyroid axis through multiple mechanisms, including interference with thyroid hormone transport protein binding, altered hepatic clearance of thyroid hormones, and alterations in their biosynthesis or action (Lopez-Espinosa et al., 2012; Weiss et al., 2009). PFAS bind to thyroid hormone transport proteins to varying degrees, depending on the compound, model system, and exposure dose. Human studies, including pregnancy and childhood cohorts, have reported associations between selected PFAS and thyroid-hormone measures, but the direction and magnitude are not uniform across compounds, trimesters, age groups, or iodine status (Lopez-Espinosa et al., 2012). This heterogeneity precludes treating thyroid effects as a uniform class response or as quantitatively equivalent to iodine deficiency.

3.3. *Hepatotoxicity and mitochondrial bioenergetic compromise*

The liver is an important target because many PFAS bind serum and hepatic proteins and can alter lipid metabolism, oxidative stress, inflammatory signaling, and mitochondrial function (Gallo et al., 2012; Ojo et al., 2020). Experimental studies report mitochondrial membrane perturbation and impaired bioenergetics at sufficiently high exposures, but relevance and compound specificity must be considered when extrapolating these findings to environmental exposures. Spatial and multi-omics approaches may help identify cell-type- and zonation-specific responses in liver, but the evidence remains emerging. Robust conclusions will require PFAS-specific datasets with spatial validation, exposure-response analysis, and independent replication before zonal susceptibility can be generalized. In the C8 Health Project/Mid-Ohio Valley population, Gallo et al. reported associations between serum PFOA or PFOS concentrations and liver-function biomarkers, including alanine aminotransferase (Gallo et al., 2012). Because this was a population with elevated PFOA exposure, the results should be interpreted within that cohort design rather than generalized automatically to nationally representative populations.

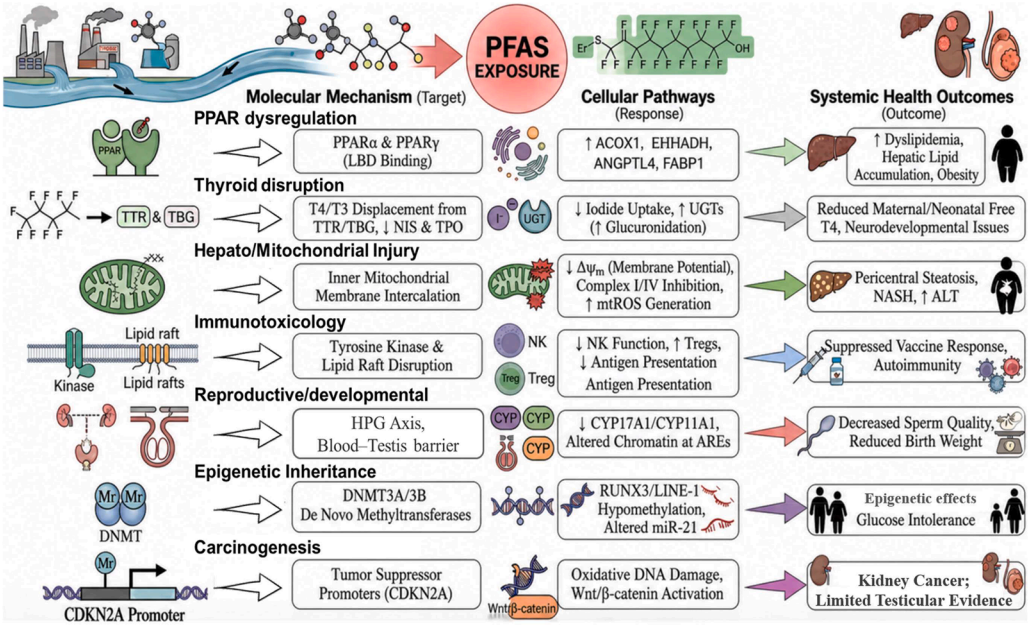

Fig. 2. Proposed mechanistic framework linking PFAS exposure to molecular targets, cellular pathways, and system-level health outcomes, including endocrine, metabolic, immunological, reproductive, epigenetic, and carcinogenic effects.

Table 2
Comprehensive summary of PFAS molecular toxicity mechanisms, affected biological targets, key quantitative evidence, and regulatory relevance.

PFAS class/compound	Primary target	Mechanistic evidence	Representative evidence and qualification	References
PFOA, PFOS, selected long-chain PFAS	Liver and lipid metabolism	PPAR modulation; altered lipid-transport and oxidative-stress pathways	Experimental receptor and gene-expression evidence; human associations with lipids and liver biomarkers, with species and confounding limitations	(Vanden Heuvel et al., 2006; Rosen et al., 2010; Nian et al., 2019; Gallo et al., 2012)
PFOA, PFOS, PFHxS and related PFAS	Thyroid axis	Transport-protein competition; altered synthesis, clearance, or signaling	Human associations are heterogeneous across compounds, age groups, pregnancy stages, and iodine status	(Lopez-Espinosa et al., 2012; Weiss et al., 2009)
PFOA, PFOS and long-chain PFCAs	Liver and mitochondria	Bioenergetic stress, lipid dysregulation, and inflammatory signaling	C8/Mid-Ohio Valley cohort associations with liver-function biomarkers; not an NHANES analysis	(Gallo et al., 2012; Ojo et al., 2020)
PFOA, PFOS and selected PFAS	Immune system	Reduced antibody responses; altered lymphocyte and antigen-presenting-cell functions	Systematic evaluations and birth-cohort evidence support reduced vaccine-antibody responses; cellular mechanisms remain endpoint-specific	(Zhang et al., 2022; Grandjean et al., 2012)
PFOA, PFOS, PFNA and mixtures	Reproductive and developmental systems	Steroidogenic, placental, and developmental signaling effects	Experimental evidence is substantial, while human semen, fertility, and birth-outcome findings remain heterogeneous	(Suramya et al., 2025; Luo et al., 2022; Impinen et al., 2019)
PFOA, PFNA and other studied PFAS	Epigenome	DNA-methylation, non-coding RNA, and chromatin changes	Human EWAS and animal studies identify exposure-associated marks; mediation and transgenerational causality are not established in humans	(Svoboda et al., 2022; Blake et al., 2020; Rashid et al., 2020; Niemiec et al., 2023; Perng et al., 2023)
PFOA; PFOS	Carcinogenesis	Oxidative stress, receptor signaling, epigenetic and immune pathways	IARC: PFOA Group 1; PFOS Group 2B. Human evidence is strongest for PFOA and kidney cancer	[(International Agency for Research on Cancer, Perfluorooctanoic Acid (PFOA) and Perfluorooctanesulfonic Acid (PFOS) 2025, Steenland et al., 2022; Barry et al., 2013)]
Legacy and replacement PFAS mixtures, including GenX, ADONA and F-53B	Multiple systems	Additive or non-additive receptor, hepatic, endocrine, and ecological responses	Mixture evidence remains composition- and endpoint-dependent; replacement PFAS requires substance-specific assessment.	(U.S. Environmental Protection Agency, 2024; Ojo et al., 2020; Sun et al., 2026)

3.4. Immunotoxicology: innate and adaptive immune suppression

Immunotoxicity is among the more consistently supported PFAS outcomes. Systematic evaluations and epidemiological studies associate PFOA and PFOS exposure with reduced antibody responses to vaccination, while experimental studies report effects on lymphocyte signaling, antigen presentation, and innate immune functions (Garvey et al., 2023; Liang et al., 2022; Zhang et al., 2022; Grandjean et al., 2012). The magnitude and persistence of these effects depend on exposure timing, compound, and host context. Changes in regulatory T-cell activity, macrophage polarization, and other immune phenotypes have been reported in experimental systems, but their direct contribution to PFAS-associated human disease remains less certain than the evidence for reduced vaccine-antibody responses. These pathways are therefore treated as mechanistic hypotheses requiring further validation rather than established population-level outcomes (Garvey et al., 2023; Liang

et al., 2022).

3.5. Reproductive and developmental toxicity

PFAS have been detected in reproductive and gestational matrices, and experimental studies indicate possible effects on steroidogenesis, Sertoli-cell integrity, placental function, and developmental signaling (Suramya et al., 2025; Blake et al., 2022; Gao et al., 2017). Epidemiological studies of semen quality and fecundity are mixed, with heterogeneity driven by differences in exposure assessment, study design, and co-exposures (Wang et al., 2023; Martinez et al., 2023; Petersen et al., 2020; Sun et al., 2023). Prenatal PFAS exposure has been associated with modest changes in birth outcomes, immune development, and neurodevelopment in some cohorts, but individual-compound associations are not uniform across studies (Govarts et al., 2016; Varsi et al., 2022; Impinen et al., 2019). Differences in exposure timing, compound mixtures, outcome definitions, covariate adjustment, and cohort composition limit causal interpretation and cross-study comparability.

3.6. Epigenetic mechanisms and transgenerational inheritance

PFAS exposure has been associated with changes in DNA methylation, non-coding RNA expression, and other epigenetic marks in experimental models and human birth cohorts (Abdulkadir et al., 2025; Liu et al., 2022; Svoboda et al., 2022; Blake et al., 2020; Rashid et al., 2020; Niemiec et al., 2023; Perng et al., 2023). These observations may help connect developmental exposure with later phenotypes, but effect sizes are generally modest, tissue specificity is incompletely resolved, and causal mediation has rarely been established. Experiments in rodents suggest that exposure-induced phenotypes may be inherited across generations, but evidence for transgenerational epigenetic inheritance must distinguish generations directly exposed during gestation from genuinely unexposed generations, and separate germline-based effects from maternal/behavioral influences (Abdulkadir et al., 2025; Liu et al., 2022; Svoboda et al., 2022). Accordingly, germline DNMT disruption should be regarded as a potential mechanism rather than a proven human outcome.

3.7. Carcinogenesis: molecular evidence and human epidemiology

IARC classified PFOA as carcinogenic to humans (Group 1) and PFOS as possibly carcinogenic to humans (Group 2B). Possible mechanisms of action include oxidative stress, receptor signaling, epigenetic modulation, and immunomodulation; however, the contribution of each is expected to vary depending on tissue and chemical type (International Agency for Research on Cancer, Perfluorooctanoic Acid (PFOA) and Perfluorooctanesulfonic Acid (PFOS) 2025). Evidence for an association between PFOA and kidney cancers is the strongest, with less evidence available for testicular cancer [(International Agency for Research on Cancer, Perfluorooctanoic Acid (PFOA) and Perfluorooctanesulfonic Acid (PFOS) 2025, Steenland et al., 2022; Barry et al., 2013)]. High-exposure studies and data from occupationally exposed populations cannot be generalized quantitatively to all PFAS or background-exposure populations.

3.8. PFAS mixture toxicity and cumulative risk assessment

Human exposure generally involves PFAS mixtures, yet most experimental and epidemiological studies remain substance-focused. Concentration-addition and mixture studies support additive or non-additive effects on hepatic, endocrine, and receptor-mediated endpoints, but mixture composition, dose range, and endpoint selection strongly influence results (Ojo et al., 2020). The 2024 U.S. drinking-water rule introduced a hazard-index approach for a defined mixture, although EPA proposed reconsideration of those provisions in 2026 (U.S. Environmental Protection Agency, 2024; U.S. Environmental Protection Agency, 2026). Regrettable substitution extends beyond PFBS, PFHxS, and HFPO-DA (GenX). ADONA and chlorinated polyfluoroalkyl ether sulfonates marketed as F-53B are prominent ether-PFAS replacements with documented environmental occurrence and incomplete toxicological characterization; F-53B is particularly relevant to electroplating activity in China (Munoz et al., 2019; He et al., 2022). Microbial communities exposed to mixed PFAS may undergo selection, functional reorganization, precursor transformation, or compound-specific partial defluorination. Engineered microbial consortia may distribute oxidative metabolism, detoxification, and fluoride tolerance among community members. However, changes in community composition or parent compound concentration alone do not demonstrate complete PFAS degradation. Verify biological transformation through transformation product identification, fluoride recovery, total organofluorine mass balance, sterile controls, and community stability assessment under environmentally realistic conditions. These considerations connect mixture toxicology with biological-remediation and outlook sections, where microbial consortia are evaluated as complementary components of integrated treatment rather than as universally validated PFAS-mineralization systems (De la Vega-Camarillo et al., 2026).

4. Current challenges in PFAS detection and remediation

The transition from toxicological evidence to environmental control involves distinguishing four processes that are commonly confused: removal from the aqueous phase, phase transfer, chemical transformation, and total mineralization. Treatment technologies must therefore be evaluated based on parent compound removal, transformation product patterns, fluoride removal, organic fluorine mass balance, matrix effects, energy and reagent requirements, residuals handling, and scalability.

4.1. Limitations of conventional water treatment

Municipal water treatment infrastructure, including coagulation/flocculation/sedimentation, sand filtration, and chlorination, was neither designed nor effective for removing dissolved ionic PFAS. Conventional coagulation processes are ineffective against PFCAs and PFSAs due to their high water solubility and anionic nature under environmental conditions (Rahman et al., 2014). Chlorination, ozonolysis, and UV irradiation are largely inert toward the C–F bond under drinking water treatment conditions. Ozone, despite its high oxidation potential (+2.1 V), does not react with the C–F bond because it preferentially reacts with electron-rich functional groups such as aromatic rings and alkenes rather than electron-deficient perfluoroalkyl chains. Granular activated carbon (GAC) is widely used for PFAS removal and can achieve high removal of selected long-chain PFCAs and PFSAs under favorable operating conditions; however, performance is strongly influenced by PFAS chain length, influent concentration, water matrix, carbon properties, and breakthrough behavior.

In contrast, GAC is less effective and shows faster breakthrough, particularly for short-chain PFAS (<C6 PFCAs, <C4 PFSAs, and neutral polyfluoroalkyl compounds), which are increasingly used as replacements and have been detected in environmental matrices. Importantly, GAC does not degrade PFAS but concentrates them on the sorbent, requiring periodic replacement or regeneration depending on influent concentration, carbon type, bed configuration, and operating conditions (Rahman et al., 2014). Ion-exchange resins can improve capture of some short-chain PFAS but generate regenerant or single-use solid waste that requires further treatment (De la Vega-Camarillo et al., 2026). Thus, these techniques should be regarded as concentration processes within treatment trains rather than as destruction processes.

4.2. Soil and sediment remediation: unique technical barriers

PFAS plumes associated with aqueous film-forming foam, industrial, landfill, or wastewater impacts can occur in heterogeneous vadose-zone and aquifer sediments, where excavation and pump-and-treat remediation are both time-consuming and costly (Brusseau et al., 2020). PFAS adsorption and transport properties are affected by organic carbon content, mineral surface area, pH, ionic strength, PFAS chain length, and precursor degradation. PFAS behavior in soil and sediment may also be influenced by biofilms and associated microbial communities. Extracellular polymeric substances can alter PFAS sorption and transport, whereas biofilm-generated redox gradients and microbial metabolism may support precursor transformation or compound-specific partial defluorination. However, decreases in aqueous parent PFAS concentrations cannot, in themselves, be interpreted as biodegradation, because adsorption to biomass or extracellular matrices may produce apparent removal. Biofilm studies should therefore include sterile or killed-biomass controls, adsorption-phase recovery, transformation product identification, fluoride measurements, and total organofluorine mass balance. Complete field-scale mineralization of saturated terminal perfluoroalkyl acids by soil biofilms has not been demonstrated. Biofilm-based strategies should currently be considered complementary components of monitored natural attenuation or hybrid physicochemical-biological treatment trains rather than stand-alone PFAS destruction technologies (De la Vega-Camarillo et al., 2026).

Regulatory monitoring at low-ng L^{-1} concentrations requires sensitive and compound-specific analytical methods. EPA Methods 533 and 537.1 use LC-MS/MS with isotopically labeled standards for defined analyte lists (U.S. Environmental Protection Agency 2024). Targeted methods therefore provide robust quantification for regulated or prioritized PFAS but cannot characterize the full inventory of known and emerging structures. Non-target high-resolution mass spectrometry can expand chemical coverage through accurate mass, isotope patterns, fragmentation, and suspect-screening libraries, although identification confidence, reference-standard availability, and quantitative comparability remain major limitations (Casey et al., 2023; Gonzalez de Vega et al., 2021; Strynar et al., 2023). Complementary measures of extractable or total organic fluorine can reveal fluorine not assigned by targeted analysis, but they do not identify individual compounds or toxicity.

4.3. Economic, institutional, and regulatory barriers

Economic and institutional barriers are substantial, and site counts require careful interpretation. Salvatore et al. mapped 57,412 presumptive PFAS contamination sites in the United States using source-based geospatial criteria; these locations were not all analytically confirmed contaminated sites and are not equivalent to the number of Superfund designations (Salvatore et al., 2022). Liabilities, dispersed monitoring, unclear residue management, and inconsistencies across country-specific standards can delay remediation decisions. The decision-making process needs to differentiate between the presumed source, scientifically proven pollution, and officially declared sites.

5. Innovative mitigation strategies: from laboratory breakthrough to field deployment

PFAS remediation technologies can be broadly classified into separation/concentration-based, destructive physico-chemical, and biological/hybrid techniques. No single technology works optimally for dilute water supplies, concentrated residues, soil, sediments, landfill leachate, and industrial wastes. Accordingly, matrix-specific treatment trains combining appropriate concentration and destructive processes may provide a practical strategy depending on PFAS composition, concentration, treatment objectives, and residual-management requirements (Fig. 3). Table 3 systematically compares the major PFAS remediation technologies across key performance dimensions.

5.1. Advanced oxidation and reduction processes

Advanced oxidation and reduction processes generate reactive species capable of initiating PFAS transformation, but reactivity depends strongly on the PFAS head group, chain architecture, solution chemistry, and whether oxidative or reductive species predominate (Lutze et al., 2018; Ren et al., 2021; Sun et al., 2025). Hydroxyl radicals alone are generally inefficient for direct attack on many perfluoroalkyl acids; sulfate radicals, hydrated electrons, and interfacial pathways can be more relevant under selected conditions. Parent-compound disappearance must be interpreted together with partial defluorination and transformation-product data. UV/sulfite and similar reduction-based processes can favor degradation in alkaline, oxygen-controlled/deoxygenated environments, while persulfate

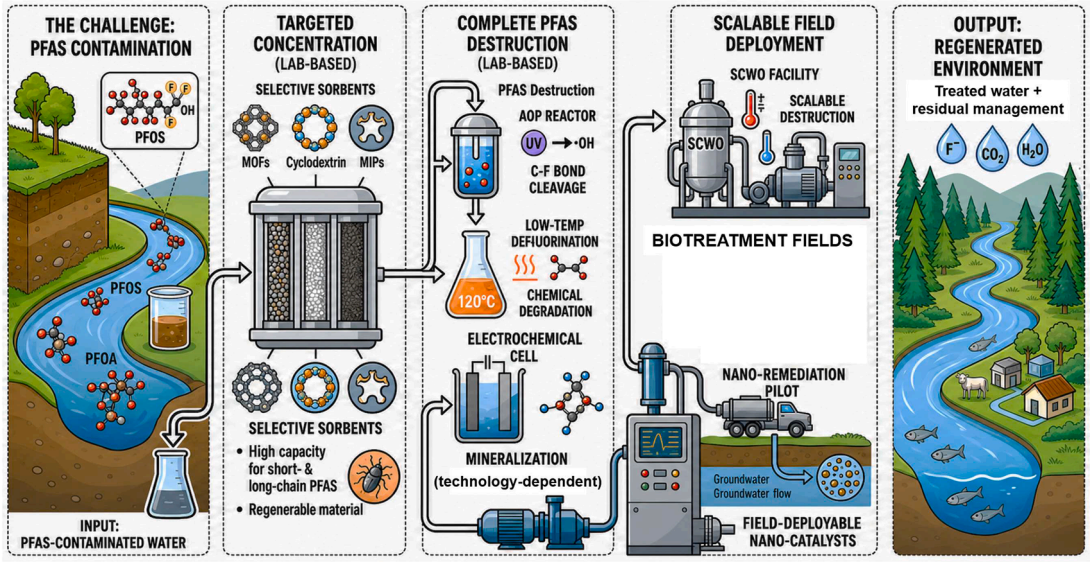

Fig. 3. Schematic overview of PFAS remediation strategies from laboratory investigation to field deployment, including separation/concentration, advanced oxidation and reduction, low-temperature chemical defluorination, electrochemical treatment, non-thermal plasma, hydrothermal/SCWO processes, advanced sorbents, nanotechnology-assisted treatment, and emerging biological approaches.

Table 3
Comparison of major PFAS remediation technologies.

Technology	PFAS/ contaminant range	Primary outcome	Defluorination/ mineralization evidence	Energy demand	Residue	Limitation	References
Granular/ powdered activated carbon (GAC/PAC)	Excellent for long-chain PFCAs/PFSAs; can treat mixed PFAS.	Separation/ concentration on carbon.	No intrinsic defluorination or mineralization	Low–moderate for adsorption; regeneration can increase energy demand	PFAS-laden carbon, regeneration off-gas, residual ash.	Short-chain breakthrough, competition from natural organic matter and regeneration.	(Jiang et al., 2024; Mortazavian et al., 2025)
Strong-base anion exchange (AIX)	Anionic PFAS, including selected short-chain compounds; capture depends on resin chemistry and hydrophobicity.	Separation/ concentration on resin	No intrinsic defluorination or mineralization	Low–moderate	Spent resin and PFAS-rich regenerant	Resin selectivity and concentrated waste management	(Jiang et al., 2024; Gao et al., 2025)
Nanofiltration / reverse osmosis (NF/RO)	Broad range of PFAS (long and short chain) separation	High rejection separation	No destruction	Moderate–high	PFAS-rich concentrate or brine	Concentrate destruction and membrane-associated PFAS contamination	(Sadia et al., 2024; Griffin et al., 2026)
UV/sulfite and related advanced reduction/ oxidation processes (ARP/ AOP)	PFCAs, PFSAs, and selected PFAS mixtures	Chemical transformation	Partial defluorination for selected PFAS	Moderate–high	Sulfite and sulfate	Electron or radical scavenging, high pH and photon attenuation	(Liu et al., 2022; Fennell et al., 2024)
Hydrothermal alkaline treatment (HALT) / low-temperature alkaline destruction	Ultrashort, short and long chain of PFAS in higher TDS solutions	Destruction along with partial defluorination	Strong fluorine mass balance	Moderate–high	Fluoride and inorganic salt	Salt handling, corrosive alkaline conditions and scale-dependent economics	(Pinkard et al., 2024; Soker et al., 2025)
Electrochemical / photo-electrochemical destruction	PFOS, PFOA and PFAS mixture	Partial defluorination and redox transformation	Destruction/ partial defluorination	Moderate–high	Fluoride, electrolyte and transformation products	Parasitic reaction, electrode fouling and energy normalization	(Guan et al., 2024; Guan et al., 2026)
Non-thermal / cold atmospheric plasma	PFSA, PFCA, PFOS and selected PFAS	Destruction or transformation	Partial defluorination	Moderate–high	Fluoride and transformation products	Gas-liquid mass transfer and reactor comparability	(Zhang et al., 2024; Kumar et al., 2026)
Advanced sorbents (cyclodextrin polymers, MOFs and related porous materials)	PFAA and PFAS	Selective concentration/ capture	No intrinsic mineralization	Low	PFAS-rich regenerant	Scale-up cost and short chain selectivity	(Lin et al., 2025; Marugán-Benito et al., 2026)
Supercritical water oxidation (SCWO)	Broad mixture of PFAS and AFFF	High temperature destruction	Destruction	High (thermal and pressure requirements)	Fluoride-containing solutions and inorganic salt	Corrosion, salt precipitation and pressure safety	(Chiang et al., 2023; Scheitlin et al., 2023; Webb et al., 2025)
Photocatalytic / solar-driven nano-enabled destruction	PFOA, PFOS and broader mixtures of PFCA and PFSA	Partial defluorination, photo-redox transformation and mineralization	Partial defluorination	Low–moderate	Catalyst, fluoride and transformation products	Catalyst recovery, long-term stability and photon penetration	(Chong et al., 2026; Liu et al., 2026)
Bioremediation / microbial consortia	Selected unsaturated PFCAs, ether-PFAS, and transformable PFAS precursors	Biotransformation	Partial defluorination for selected PFAS	Low	Biomass, transformation products and fluoride-containing effluent	Specificity, slow kinetics and high PFAS concentration	(De la Vega-Camarillo et al., 2026; Xu et al., 2025)

activation methods have shown variable efficiencies on a case-by-case basis (Lutze et al., 2018; Ren et al., 2021; Cheng et al., 2010). Most high removal rates have been achieved either in laboratory experiments or at concentrations higher than drinking water. Reagent consumption, scavenging effects, sulfate or sulfite residuals, and poor fluoride recoveries remain major scale-up limitations.

5.2. Low-temperature chemical defluorination of PFCAs

Trang et al. reported the mineralization of selected perfluorocarboxylic acids at low temperatures using polar aprotic solvents and sodium hydroxide at approximately 120°C. The process takes advantage of head-group activation and applies primarily to concentrated PFCA waste streams, not directly to dilute drinking water. The applicability to perfluoroalkyl sulfonates, ether-based PFAS, complex environmental matrices, solvent recovery, reagent use, and continuous-flow operation remains uncertain and requires further investigation. Combining a concentration process with low-temperature treatment is technically appealing, but its economic efficiency depends on solvent recovery, waste stream composition, scale, reagent reuse, and

destruction. Economic studies must report results in terms of the cost per 1,000 US gallons of the defined feed stream and include energy consumption, solvent losses, handling of byproducts, and treatment of residuals (Trang et al., 2022).

5.3. Electrochemical mineralization

Electrochemical oxidation using suitable high-overpotential anodes can promote PFAS transformation and, under appropriate conditions, fluoride release through direct electron-transfer and interfacial reaction pathways (Radjenovic and Sedlak, 2015; Zhuo et al., 2011). Electrochemical efficiency depends on current density, conductivity, mass transfer, electrode material, co-contaminant presence, and PFAS concentration. High removal rates do not necessarily indicate mineralization. An electrochemical process is most favorable for concentrated effluents, brine, or final polishing steps when the system conductivity and hydrodynamics can be well controlled. The reported energy consumption varies widely across studies and must be normalized by treated volume, PFAS removal, and fluoride ion recovery. The parameters discussed are valid for optimization; however, AI-controlled utility-scale electrochemical process performance for PFAS remains unknown.

5.4. Non-thermal plasma treatment

Non-thermal plasma reactors generate electrons, photons, radicals, and reactive interfacial species without heating the entire water volume to thermal-plasma temperatures. Reverse-vortex gliding-arc plasma has degraded PFOA, PFOS, and other PFAS in laboratory aqueous systems, with performance influenced by chain length, gas-liquid mass transfer, conductivity, and background organic matter (Lewis et al., 2020). Plasma appears highly promising for removing PFAS enriched at the gas-liquid or bubble interface; however, energy input and reactor design complicate direct comparisons among studies. Plasma-jet treatment under cold atmospheric pressure was shown to transform short-chain PFCAs, PFSAs, GenX, and ADONA, along with specific byproducts (Topolovec et al., 2024). This supports considering plasma as one of several technologies warranting continued development, while also showing that removal, partial defluorination, and full mineralization are distinct goals. Pilot-scale treatment of real concentrates, fluorine mass balance, off-gas characterization, and energy-normalized benchmarking remain priorities.

5.5. Engineered sorbent materials: Metal-organic frameworks (MOFs), cyclodextrin polymers, and molecularly imprinted polymers (MIPs)

Engineered sorbents aim to improve affinity, kinetics, or selectivity beyond those of conventional activated carbon. Metal-organic frameworks, ionizable polymers, cyclodextrin networks, and molecularly imprinted systems can exploit hydrophobic, electrostatic, and host-guest interactions with PFAS (FitzGerald et al., 2022; Lee et al., 2025; Li et al., 2022; Zhang et al., 2025). Maximum reported capacities depend significantly on test concentration, water chemistry, competing organics, and normalization methods, so they cannot be directly compared. Regeneration, irreversible fouling, mechanical stability, leaching, manufacturing cost, and management of PFAS-rich regenerants determine whether advanced sorbents can progress beyond laboratory demonstrations. Their most credible role is selective concentration followed by a verified destructive step.

5.6. Supercritical water oxidation and hydrothermal alkaline treatment

Supercritical water oxidation can achieve high destruction and removal efficiency (DRE) for concentrated PFAS solutions at high temperatures and pressures (Scheitlin et al., 2023; Webb et al., 2025). Its strengths include broad organic destruction and applicability to concentrated waste streams, whereas major limitations include high capital and energy requirements, corrosion, salt precipitation, and the need for comprehensive characterization of fluoride, gaseous emissions, and persistent transformation products. The process performance should be characterized for each PFAS type.

5.7. Nanotechnology-enhanced remediation

While nanomaterials can enhance adsorption/separation/electrochemical/photochemical processes, the term “nano-remediation” encompasses mechanisms at varying levels of development (Wang et al., 2026; Mahpishanian et al., 2024). Magnetic composite materials could help with sorbent recovery, while photocatalysts could convert certain PFAS under optimized conditions. Evidence is presently insufficient to conclude that nanoscale zero-valent iron mineralizes terminal PFAS under field conditions; thus, it should be regarded primarily as an agent for redox condition modification rather than a destruction mechanism of PFAS.

5.8. Bioremediation frontiers

Biological PFAS remediation should be described in terms of demonstrated transformation and measured partial defluorination rather than an absolute claim that microorganisms cannot cleave C-F bonds. Anaerobic enrichments have succeeded in transforming and partially defluorinating some selected unsaturated and ether-containing PFAS, while terminally saturated forms of PFOA and PFOS appear to be more refractory under most environmental conditions (Xu et al., 2025; Khan and Murphy, 2023; Khan et al., 2023). One study from 2026 demonstrated rapid degradation and release of GenX-derived fluoride using either selected or genetically engineered bacteria; however, independent corroboration is necessary (De la Vega-Camarillo et al., 2026). Evidence also suggests a potential role for fungal systems in PFAS transformation. For example, *Cunninghamella elegans* has been reported to transform 6:2 fluorotelomer alcohol through cytochrome P450-mediated metabolic pathways (Khan and Murphy, 2023). Fungal cytochrome P450 enzymes may also participate in the metabolism of structurally diverse xenobiotic substrates.

The combination of photocatalytic degradation and subsequent fungal degradation resulted in enhanced PFOA degradation and partial defluorination compared to each treatment alone in a high-concentration laboratory setup (Khan et al., 2023). Microbial consortium and biofilm techniques can distribute oxidative metabolism, detoxification, and fluoride tolerance among various microorganisms, although incomplete mineralization, inhibitory compounds, and sluggish kinetics are significant hurdles (De la Vega-Camarillo et al., 2026). As such, biological processes are currently best suited to serve as transformative steps within a treatment train as part of a larger solution for precursors and certain ether- or unsaturated-PFAS-containing compounds. Future studies should include sterile and sorption controls, isotope or mass-balance confirmation, fluoride recovery, non-target product analysis, community stability, and tests in soil, groundwater, leachate, or wastewater matrices at realistic concentrations.

6. AI and machine learning applications: evidence levels, current use, and future opportunities

AI/ML applications relevant to PFAS research span a wide range of evidentiary maturity. To distinguish between demonstrated applications, transferable methodologies, and prospective concepts, we classify the evidence throughout this section into three levels. Level A denotes PFAS-specific modeling or experimental applications supported by verifiable PFAS data; Level B denotes methods established in adjacent fields such as chemistry, materials science, environmental engineering, or water treatment but not yet validated at the claimed scale for PFAS; and Level C denotes prospective or conceptual applications that require

substantial PFAS-specific data, experimental validation, or technological development. These evidence levels are applied consistently throughout (Abdulkadir et al., 2025–Niemiec et al., 2023) and summarized in Table 4.

6.1. Quantitative structure–activity relationship (QSAR) modeling and GNNs for toxicity prediction across the PFAS universe

Classical QSAR and machine-learning models relate molecular descriptors or fingerprints to bioactivity, physicochemical properties, or environmental behavior. PFAS datasets can draw on EPA high-throughput bioactivity resources, published studies, and curated chemical inventories, but endpoint coverage remains sparse and structurally biased. Because ToxCast releases may differ in their numbers of assays, assay components, and endpoints, PFAS modeling studies should report the exact data release, endpoint definitions, chemical identifiers, inclusion criteria, and access date (U.S. Environmental Protection Agency, 2025).

Graph neural networks and pretrained molecular representations can reduce manual descriptor selection, but they do not eliminate small-sample bias, label noise, or applicability-domain problems (Ye et al., 2026; Yang et al., 2019). Reported internal cross-validation can overestimate performance when close structural analogs occur in both training and test sets. Scaffold-aware or cluster-aware splits, external validation, uncertainty calibration, and transparent endpoint definitions are therefore essential before regulatory use. Active learning can prioritize chemicals whose testing is expected to reduce model uncertainty, but published demonstrations cited here are primarily methodological or from adjacent discovery domains rather than validated reductions in PFAS testing effort (Reker and Schneider, 2015). For PFAS, the near-term value is a testable prioritization workflow linking model uncertainty to high-throughput assays, not a prespecified five- or ten-fold efficiency claim.

Evidence status Level A/B: PFAS-specific descriptor-based and machine-learning toxicity models have been reported, providing direct evidence that these approaches can be applied to PFAS datasets. However, limited sample sizes, heterogeneous endpoint definitions, structural bias, and insufficient external validation prevent these approaches from being considered uniformly mature across the broader PFAS chemical space.

6.2. Multi-omics data fusion and systems-level toxicology

Multi-omics methods such as MOFA+ and network analysis can integrate transcriptomic, epigenomic, proteomic, or metabolomic data, but they require matched samples, adequate replication, and careful control of batch and exposure variables (Langfelder and Horvath, 2008; Argelaguet et al., 2018). In PFAS toxicology, these methods are most useful for generating reproducible pathway hypotheses and candidate biomarkers; they should not be presented as proof that a specific regulatory factor or therapeutic intervention has been established unless supported by the underlying PFAS dataset.

Evidence status Level A/B: PFAS-specific transcriptomic, epigenomic, proteomic, and metabolomic datasets provide direct evidence for omics-based toxicological investigation; however, matched-sample multi-omics integration, independent replication, tissue-resolved validation, and causal interpretation remain comparatively limited. For PFAS multi-omics, reproducibility depends on complete metadata, explicit exposure concentrations, transparent preprocessing, factor stability, and independent biological validation. Distinguish general integration methods or network-medicine tools from PFAS-specific applications, and treat inferred regulatory modules as hypotheses until targeted experiments support them.

6.3. Generative AI for safer fluorochemical design: breaking the regrettable substitution cycle

Currently, generative design of PFAS alternatives is an in silico research concept rather than a validated route to safer fluorochemicals. Computational models can propose structures that optimize predicted functionality, persistence, or toxicity objectives, but these objectives inherit the limitations of the training data and property predictors (Wang et al., 2026).

Evidence status Level C: Generative molecular design for safer

Table 4
Evidence-calibrated summary of AI/ML applications relevant to PFAS research.

AI/ML method	Potential PFAS application	Current evidence status	Key limitations and validation needs	References
Descriptor-based ML and GNNs	Toxicity or property prediction	Level A/B: PFAS-specific studies exist, but datasets are small and endpoints heterogeneous	External, structure-aware validation; uncertainty; curated labels; defined applicability domain	(Ye et al., 2026; Yang et al., 2019)
Active learning and Bayesian optimization	Testing prioritization	Level B: established methodology; limited closed-loop PFAS validation	Prospective experimental cycles and predefined stopping criteria	(Reker and Schneider, 2015)
Multi-omics integration	Systems toxicology and biomarker discovery	Level A/B: PFAS omics data exist; integrative analyses remain limited by matched-sample availability	Batch correction, causal interpretation, tissue resolution, and replication	(Langfelder and Horvath, 2008; Argelaguet et al., 2018)
Generative molecular design	Candidate safer alternatives	Level C: computational proposals exist, but safer functional replacements cannot be established without synthesis and experimental validation	Synthetic feasibility, performance, persistence, degradability, and multi-endpoint toxicity validation	(Wang et al., 2026)
Digital twins and physics-informed models	Treatment-process simulation and optimization	Level B: water-treatment demonstrations exist; PFAS-specific full-scale validation is not established	Pilot operational data, calibrated kinetics, residuals and mass balance, fail-safe control	(Ma et al., 2025; Venkata Siva Prakash, 2019; Croll et al., 2023)
Reinforcement learning	Adaptive process control	Level B/C: established in adjacent process-control applications, but PFAS-specific deployment remains largely prospective	Safe offline training, regulatory constraints, out-of-distribution detection, operator override	(Croll et al., 2023)
Self-driving laboratories	Sorbent, catalyst, or condition discovery	Level B: autonomous chemistry platforms are established; cited work was not a PFAS demonstration	Standardized PFAS assays, contamination control, analytical throughput, provenance	(Roch et al., 2018)
Sensor data analytics	Signal processing and anomaly detection	Level A/B: PFAS sensor research exists; continuous field networks remain limited	Selectivity, drift, matrix effects, false alarms, and reference-method confirmation	(Liang et al., 2025; Chugh et al., 2026; Ahmadi Tabar et al., 2024)
Geospatial statistical and ML models	Source screening and monitoring prioritization	Level A/B: source-occurrence models exist; predictions require ground-truth validation	Ground-truth sampling, spatial transferability, uncertainty, and distinction between presumptive and confirmed contamination	(Hu et al., 2016; Salvatore et al., 2022)

PFAS alternatives remains a prospective computational application. Predicted candidates cannot be considered safer or more environmentally preferable until they undergo synthesis, structural confirmation, functional performance testing, persistence and transformation assessment, bioaccumulation evaluation, and multi-endpoint toxicological validation. Computationally generated alternatives must not be described as safer solely based on predicted scores. Comparisons with legacy PFAS should include uncertainty and applicability-domain analysis for every property model.

6.4. Digital twin simulation and RL for remediation optimization

Digital twins combine mechanistic process models, operational data, sensors, and surrogate models to evaluate treatment scenarios (Ma et al., 2025; Venkata Siva Prakash, 2019; Croll et al., 2023). This approach is established in parts of water and manufacturing engineering, but a fully calibrated PFAS treatment digital twin integrating adsorption, destruction, transformation products, fluorine mass balance, and residuals management has not yet been demonstrated at utility scale.

Evidence status Level B: Digital-twin frameworks are established in water-treatment and process-engineering applications and are technically transferable to PFAS remediation. However, a fully calibrated PFAS-specific digital twin integrating adsorption, destruction kinetics, transformation products, fluorine mass balance, residual management, and field-scale operational data has not yet been validated at utility scale. Potential PFAS applications of digital twins include sensitivity analysis, pilot-plant design, uncertainty propagation, and comparison of treatment-train configurations. Performance estimates should be explicitly labeled as simulated, pilot-derived, or field-validated, and should state the baseline, system boundary, influent composition, treatment objective, and uncertainty range.

Reinforcement learning may eventually support adaptive process control, but PFAS-specific deployment would require constrained policies, out-of-distribution detection, operator override, regulatory failsafes, and validation under changing influent composition. Evidence transferred from adjacent wastewater-control studies should be treated as methodological precedent rather than as a demonstrated PFAS cost reduction, energy, or performance improvement (Croll et al., 2023).

Evidence status Level B/C: Reinforcement learning is established as a process-control methodology in adjacent wastewater and engineering applications, but PFAS-specific adaptive-control demonstrations remain largely prospective. Safe deployment would require constrained policies, out-of-distribution detection, override operators, regulatory safeguards, and validation under changing PFAS mixtures and influent conditions.

6.5. Autonomous robotic laboratories and high-throughput PFAS screening

Self-driving laboratories integrate automation, analytics, and iterative experimental design, and have accelerated discovery across other materials and chemical domains. For PFAS research, plausible applications include sorbent screening, catalyst composition, electrochemical conditions, and biological-consortium optimization. These applications remain prospective until closed-loop PFAS studies demonstrate reproducible gains against predefined analytical and treatment benchmarks. A credible PFAS autonomous workflow would require contamination-resistant robotics, validated fluoride and organofluorine analytics, non-target byproduct identification, complete data provenance, and confirmation at environmentally relevant concentrations. Until PFAS-specific closed-loop campaigns are reported, ChemOS and related platforms should be viewed as transferable experimental infrastructure rather than demonstrated PFAS-remediation systems (Roch et al., 2018).

Evidence status Level B: Autonomous and self-driving laboratory platforms are established in chemistry and materials discovery, demonstrating the feasibility of closed-loop experimentation. However, their PFAS-specific use as sorbents, catalysts, electrochemical conditions, or biological consortia remains insufficiently validated through reproducible closed-loop PFAS campaigns.

6.6. AI-Integrated environmental monitoring and real-time surveillance networks

Optical, electrochemical, immunochemical, aptamer, and imprinted-polymer sensors are being developed for PFAS detection, and machine learning can assist signal processing, classification, calibration transfer, and drift detection (Liang et al., 2025; Chugh et al., 2026; Ahmadi Tabar et al., 2024). However, sensitivity reported in buffers does not establish selectivity or quantitative reliability in drinking water, wastewater, food, or serum. Continuous networks require routine confirmation using standardized mass spectrometric methods. **Evidence status Level A/B:** PFAS-specific optical, electrochemical, immunochemical, aptamer-based, and molecularly imprinted sensing studies provide direct evidence for sensor development and data-assisted signal interpretation. However, continuous field-scale AI-enabled monitoring remains limited by matrix effects, sensor drift, selectivity, false-positive control, calibration transfer, and the continuing need for mass-spectrometric confirmation. Geospatial models can combine monitoring records with locations of industrial facilities, military sites, airports, wastewater infrastructure, land use, and hydrogeology to prioritize sampling (Hu et al., 2016; Salvatore et al., 2022). Satellite imagery may contribute to land-cover or watershed covariates, but satellites do not directly measure dissolved PFAS. Establish geospatial model performance using spatially independent validation, calibrated uncertainty, and prospective testing at out-of-sample monitoring sites. Geospatial prediction cannot replace LC-MS/MS analysis for confirming contamination but should be used to identify data gaps and guide confirmatory sampling.

Evidence status Level A/B: PFAS-specific source-occurrence and geospatial models have been used to support contamination screening and sampling prioritization. Nevertheless, these models require spatially independent validation, uncertainty calibration, and prospective field confirmation and should not be interpreted as direct measurements of PFAS contamination.

6.7. Explainable AI (XAI) and regulatory acceptance of ML predictions

A key, though often neglected, aspect of deploying AI/ML technologies in PFAS research is the explainability of predictions and their regulatory acceptability (Fig. 4). Regulatory frameworks such as EPA TSCA risk evaluations and ECHA REACH SVHC require transparent mechanistic reasoning for hazard conclusions, which black-box deep learning models cannot provide (Murdoch et al., 2019). XAI methods address this gap. For instance, gradient-weighted class activation mapping (Grad-CAM) for molecular graphs helps identify the key atomic substructures that contribute most to toxicity predictions. Similarly, SHapley Additive exPlanations (SHAP) quantify the contribution of individual molecular features to model outputs, which can be interpreted from a chemical perspective. Finally, attention mechanism visualization in transformer-based models helps identify the key molecular fragments and interactions that are most strongly weighted in activity predictions (Murdoch et al., 2019). The OECD QSAR principles, EPA new-approach-method discussions, and related regulatory frameworks emphasize defined endpoints, transparent algorithms, validation, applicability domains, and mechanistic interpretation (Ye et al., 2026; Murdoch et al., 2019; Zhong et al., 2021). The EPA ToxCast resource contains high-throughput bioactivity data, but ML outputs remain a single line of evidence in a weight-of-evidence assessment rather than automatic regulatory determinations.

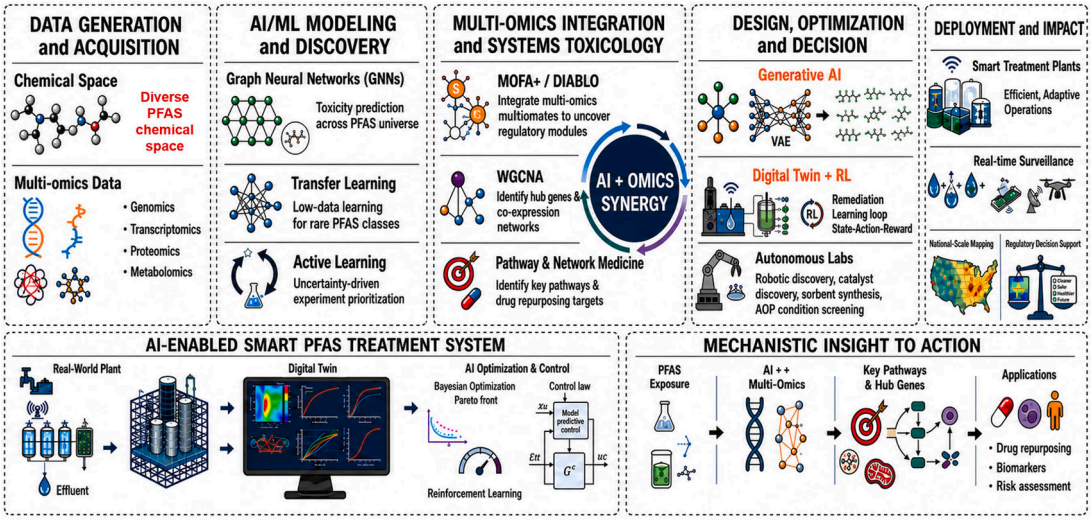

Fig. 4. AI and multi-omics integration roadmap for PFAS research, illustrating a workflow from data generation and AI/ML discovery through multi-omics systems toxicology, design and optimization, and deployment and impact, with an integrated smart PFAS treatment system linking mechanistic insight to action for safer remediation, ecosystem protection, and policy support.

6.8. AI-assisted enzyme discovery and protein engineering for PFAS biotransformation

AI-assisted enzyme engineering is best categorized as a Level B/C research opportunity rather than a validated PFAS-remediation technology. Protein models, structure-prediction tools, sequence-function models, and active learning workflows can prioritize fungal, microbial, or metagenomic enzymes and variants for experimental assessment (Stockbridge and Wackett, 2024; Marciesky et al., 2023). However, predicted binding or broad xenobiotic activity does not reveal catalytic C-F bond cleavage. PFAS-specific validation should include purified enzyme turnover assays, identification of transformation products, fluoride recovery, total organofluorine mass balance, and testing in environmentally realistic matrices (Wackett, 2025).

7. Outlook: The PFAS Nexus as an evidence-to-decision framework

Established evidence, transferable methods, and long-horizon concepts are separated explicitly so that future-looking ideas do not acquire the status of demonstrated PFAS technologies.

7.1. Circular fluorine economy and sustainable fluorochemistry

Long-term PFAS management requires prevention, substitution, and treatment. A circular-fluorine perspective may include recovery of inorganic fluoride from verified destruction processes, product redesign, essential-use assessment, life-cycle analysis, and extended producer responsibility (Yang et al., 2025; Long et al., 2026). However, recovery routes, product quality, energy demand, and market feasibility require case-specific evaluation; fluorine cannot be assumed to be economically recoverable from every treatment stream. AI may support multi-objective screening of candidate alternatives, but life cycle and hazard constraints must be based on measured or validated data. The framework should penalize persistence, transformation into hazardous products, and regrettable substitution, rather than optimizing a single functional property.

7.2. Synthetic biology and fluorinase engineering for biological C–F bond cleavage

Biological C-F bond cleavage is no longer appropriately described as impossible in all PFAS contexts. Partial defluorination has been reported for selected unsaturated and ether-containing PFAS, and designed microbial consortia have recently shown promising GenX transformation and fluoride release (Yu et al., 2022; De la Vega-Camarillo et al., 2026). These findings do not establish broad mineralization of saturated PFOA, PFOS, or the full PFAS class. Fluorinase catalyzes biological C-F bond formation, not the reverse cleavage of PFAS, and engineering a general PFAS defluorinase remains a long-term hypothesis (O'Hagan and Deng, 2015). A more evidence-grounded near-term program would combine metagenomic enzyme discovery, purified-enzyme assays, isotope and fluoride mass balance, microbial-consortium design, and hybrid biological-physicochemical treatment. ML-guided protein engineering can help prioritize variants, but catalytic turnover must be demonstrated experimentally.

7.3. Long-horizon computational chemistry

High-level quantum chemistry can improve understanding of bond activation, radical intermediates, and catalyst mechanisms. Quantum computing may eventually complement classical electronic-structure methods, but current applications to PFAS reaction systems remain exploratory (Babbush et al., 2018). Testing its value must focus on reproducible chemical accuracy and computational advantage in PFAS-relevant reactions, not hardware size or deployment schedules. Near-term priorities are improved classical calculations, experimentally benchmarked reaction pathways, open kinetic datasets, and uncertainty-aware surrogate models. Quantum algorithms should remain an outlook topic until they demonstrate reproducible advantage for chemically relevant PFAS systems.

7.4. Policy–technology interface and the role of AI in regulatory science

AI/ML might help screen for relevant evidence, identify chemicals of concern, design sampling plans, and conduct scenario assessments, but regulation will need transparent data lineage, uncertainty quantification, validation, and human oversight. Models of source-occurrence relationships could inform sampling locations; they do not provide measurements or assign liability. International harmonization would be aided by substance nomenclature, machine-readable study metadata, consistent endpoint definitions, and benchmarking datasets.

8. Conclusions, future perspectives, and priority research actions

This review integrates PFAS toxicology, remediation, and emerging AI/ML applications while explicitly calibrating claims to the strength of the evidence. Toxicological concerns are well supported for several legacy PFAS, but the available evidence is uneven and cannot be generalized to all compounds captured by expanding structural inventories. Remediation performance is likewise matrix- and endpoint-dependent: adsorption and membranes concentrate PFAS, whereas electrochemical, plasma, thermal, photochemical, chemical, and biological approaches differ in their ability to transform, defluorinate, or mineralize specific compounds. No technically complete, universally applicable PFAS treatment train has yet been established. Integrated systems that combine selective concentration with destructive treatment are promising, but require fluorine mass balance, byproduct evaluation, residuals management, energy and cost analysis, and pilot-to-field validation. Biological remediation is an important complementary frontier, especially for precursors, ether-PFAS, and hybrid processes, although complete and reproducible mineralization of saturated terminal PFAS remains a major challenge. AI/ML currently offers its clearest PFAS value in data curation, chemical prioritization, interpretable prediction, experimental design, and monitoring support. Digital twins, self-driving laboratories, generative alternatives, and ML-guided enzyme engineering are credible research directions, but most are not yet validated as PFAS-specific field solutions.

Priority research actions

1. Develop open, FAIR PFAS datasets with explicit substance identifiers, study quality metadata, negative results, and externally usable toxicity and treatment endpoints.
2. Require parent-compound analysis, transformation-product identification, fluoride recovery, and total-organofluorine mass balance in destructive-treatment studies.
3. Evaluate integrated concentration-destruction treatment trains in realistic matrices and report energy, residuals, and costs using clearly defined units such as USD per 1,000 US gallons.
4. Expand controlled studies of fungal systems, biofilms, anaerobic cultures, and synthetic microbial consortia, with independent replication and reactor-scale validation.
5. Benchmark PFAS ML models using structure-aware external splits, uncertainty calibration, applicability-domain reporting, and prospective experimental tests.
6. Develop harmonized evidence and reporting standards that distinguish laboratory proof-of-concept, pilot demonstration, field validation, and regulatory acceptance.

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Declaration of competing interest

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

Data availability

No data was used for the research described in the article.

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