

Mechanistic Insights, Molecular Modeling, and Material Design in Wastewater Treatment through Computational Approaches

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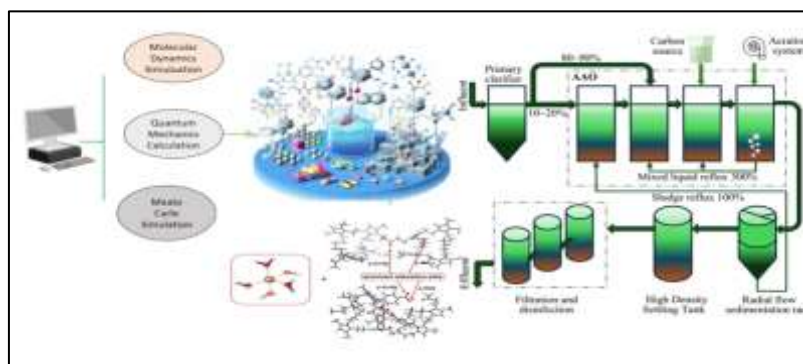
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Abstract



Graphical Abstract

Computational chemistry is becoming a key tool for comprehending and creating new treatment materials due to the growing need for sustainable and effective wastewater treatment methods. This study thoroughly examines the molecular modeling, material design techniques, and mechanistic insights that support the creation of novel wastewater treatment solutions. Researchers can decipher the molecule-level adsorption, degradation, and catalytic processes of pollutants by utilizing density functional theory (DFT), molecular dynamics (MD) simulations, and quantum chemistry computations. In addition to making it easier to identify active sites and reaction pathways, these insights also make it possible to rationally design functional materials with improved specificity and efficiency, such as metal-organic frameworks (MOFs), covalent organic frameworks (COFs), graphene-based composites, and photocatalysts. The optimization of structural and electrical characteristics is made possible by molecular modeling, which also helps forecast the physicochemical interactions between pollutants and treatment materials. Furthermore, machine learning integration and computational screening are becoming effective strategies for speeding up the search for new therapeutic ingredients. Recent developments in computational methods for wastewater treatment are summarized in this study, emphasizing the cooperation between theoretical forecasts and experimental confirmations. The focus is on how computational insights drive process optimization and material innovation in the removal of new pollutants, heavy metals, dyes, and medicines. To create next-generation materials for water purification, the paper ends by describing upcoming potential and difficulties in combining data-driven design, multiscale simulations, and green chemistry principles. This integrated computational method has the potential to transform wastewater treatment technology and advance public health and environmental sustainability.

Keywords: Computational Chemistry, Wastewater Treatment, Molecular Modeling, Mechanistic Insights, Material Design, Density Functional Theory (DFT), Adsorption Mechanisms, Advanced Oxidation Processes, Catalysis in Water Purification, Quantum Chemical Simulations, Contaminant Degradation Pathways.

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INTRODUCTION

Advanced wastewater treatment is becoming more and more necessary as urban populations rise and industrial activity increases (Zhang *et al.*, 2016). The complex cocktail of contaminants that today contaminate urban and industrial wastewater streams, including heavy metals, pharmaceutical residues, microplastics, and new organic pollutants, is becoming more and more difficult to treat using traditional treatment technologies (Baig *et al.*, 2024). To guarantee that discharged water satisfies strict environmental regulations, modern wastewater treatment technologies such as membrane filtration, activated carbon adsorption, advanced oxidation processes, and biological nutrient removal are crucial. Beyond just maintaining water quality, advanced treatment systems are essential for fostering environmental sustainability because they protect public health, stop aquatic ecosystems from deteriorating, and allow treated water to be reused for industry, agriculture, or even drinking. Additionally, by collecting energy and nutrients from waste streams, these systems promote the circular economy. Investing in improved wastewater treatment is now essential to sustainable development plans due to climate change, water shortages, and growing environmental laws. In addition to being a necessity for the environment, it offers a chance for innovation, resource conservation, and the construction of robust water infrastructure for coming generations (Tehseen *et al.*, 2024).

In the current day, traditional treatment techniques for dealing with environmental contaminants and creating new materials still confront some significant obstacles (Ullah *et al.*, 2024). These traditional methods, which frequently depend on empirical research and trial-and-error approaches, are frequently laborious, resource-intensive, and have a limited ability to forecast and control intricate molecular interactions. Traditional chemical or physical remediation techniques may not be able to adequately address persistent or developing pollutants in pollutant degradation, such as heavy metals, pharmaceutical residues, and microplastics, which require precise and flexible methodologies (Liu *et al.*, 2024). Furthermore, traditional material design frequently finds it difficult to meet the increasing need for high-performance, sustainable, and multifunctional materials, especially in industries like environmental engineering, biomedicine, and energy storage. Consequently, the value of computational methods in environmental cleanup and material innovation is becoming more widely acknowledged. Molecular dynamics simulations, density functional theory (DFT), and machine learning algorithms are examples of computational techniques that enable researchers to accurately and efficiently simulate, screen, and optimize materials at the atomic and molecular levels (Sibanda *et al.*, 2022). These methods make it possible to forecast the characteristics of materials, make it easier to find new compounds with particular uses, and aid in the

comprehension of intricate pollution-degrading processes. Scientists can speed up the creation of smart materials and catalytic systems that can more selectively and sustainably break down contaminants by combining computational modeling with experimental data. This will open the door to more sophisticated solutions to pressing environmental and technological issues (Porter *et al.*, 1995).

Because computational chemistry makes it possible to precisely model and simulate molecular systems, it is essential for tackling difficult problems in contemporary chemical, biological, and materials sciences (Kollman *et al.*, 1996). Fundamentally, computational chemistry uses statistical techniques, quantum mechanics, and molecular mechanics to forecast the structure, behavior, and reactivity of molecules, providing a productive and economical substitute for conventional experimental methods. Molecular modeling, which enables researchers to accurately mimic molecular interactions, binding affinities, and reaction pathways, is one of the most revolutionary uses (Honarparvar *et al.*, 2014). Understanding how drug candidates interact with their biological targets helps speed up the development of new treatments while reducing the need for expensive laboratory testing, which is especially useful in drug design. To identify lead compounds and optimize their attributes, molecular dynamics simulations and docking studies help forecast how a molecule would interact in a complicated biological context. Additionally, by forecasting molecule configurations, electrical characteristics, and stimulus response, computational chemistry in material science helps to build smart materials and catalysts (Jablonka *et al.*, 2020). Molecular modeling is set to broaden its predictive reach as computing capacity and algorithmic complexity increase, providing a more profound understanding of protein-ligand interactions, allosteric modulation, and solvation effects. In the end, computational chemistry facilitates innovation in a variety of scientific fields by acting as a fundamental instrument for hypothesis creation and confirmation.

Mechanistic Insights into Wastewater Treatment Processes

Adsorption and Degradation Mechanisms

The removal of environmental pollutants, especially in water treatment applications that target dyes, pharmaceuticals, and per- and polyfluoroalkyl substances (PFAS), depends heavily on adsorption and degradation processes (Merino *et al.*, 2014). The main process of adsorption is the physical or chemical binding of contaminants to the surface of materials like metal-organic frameworks (MOFs), biochar, activated carbon, or nanocomposites. Drugs such as diclofenac or carbamazepine, for example, are efficiently adsorbed on graphene oxide or carbon nanotubes through π - π interactions, hydrogen bonds, and electrostatic attractions. Van der Waals forces, ionic interactions, and

surface area availability all play a role in the comparable adsorptive behavior of dyes like methylene blue and rhodamine B onto mesoporous materials and biopolymers. Degradation processes are essential for thorough cleanup since adsorption by itself cannot eliminate pollutants (Mudhoo *et al.*, 2019). Complex chemical molecules are broken down into simpler, frequently innocuous substances during degradation, particularly oxidative degradation. Fenton and Fenton-like reactions are examples of advanced oxidation processes (AOPs) that work very well. In traditional Fenton systems, hydrogen peroxide (H_2O_2) and ferrous iron (Fe^{2+}) combine to form hydroxyl radicals ($\bullet\text{OH}$), which oxidize pollutants in a non-selective manner. Heterogeneous catalysts like iron-containing clays, Fe_3O_4 , or zero-valent iron (ZVI) can increase radical production and prolong reaction efficiency across a wider pH range in Fenton-type systems. For instance, using ESR spectroscopy and scavenger tests, a case study employing a magnetite-supported Fenton-like catalyst showed that hydroxyl radicals were involved in the over 90% degradation of ciprofloxacin in aqueous medium within 30 minutes. Similar to this, sophisticated procedures like electrochemical oxidation or AOPs based on sulfate radicals (such as peroxymonosulfate activation) can break the strong C–F bonds in PFAS breakdown. In a noteworthy work, PFOS was degraded using cobalt-doped biochar as a peroxymonosulfate activator. LC-MS analysis revealed a radical-based defluorination route. The significance of combining adsorption with sophisticated degrading techniques to guarantee thorough pollutant removal and environmental safety is highlighted by the fact that these pathways frequently entail sequential oxidation, bond-breaking, and mineralization processes (Zou *et al.*, 2023).

Catalytic Pathways for Pollutant Removal

A crucial area of environmental remediation is the elimination of pollutants by catalytic pathways,

which use both homogeneous and heterogeneous catalytic systems to break down or convert dangerous pollutants into safe byproducts (Waclawek *et al.*, 2018). High thermal stability, ease of separation, and reusability are benefits of heterogeneous catalysts, which are usually solid substances that function in separate phases from the contaminants (such as metal oxides, zeolites, or supported noble metals). These systems frequently work by activating reactive oxygen species (ROS), such as superoxide and hydroxyl radicals, which destroy organic contaminants violently, as well as via surface-mediated redox processes and adsorption. On the other hand, more uniform contact and precise reaction control are made possible by homogeneous catalysts, in which the pollutant and catalyst share the same phase, often liquid. Transition metal complexes or organic catalysts are frequently used to achieve high reaction specificity and rates. The creation of sophisticated homogeneous catalysts has made it possible to fine-tune degradation processes, especially in moderate environments. Using natural or modified enzymes such as laccases, peroxidases, and oxygenases, enzymatic degradation models a subset of biocatalysis, provides a highly selective and environmentally friendly substitute (Bassanini *et al.*, 2020). Mechanistic investigations of these enzymes provide insights into substrate binding, active site design, and catalytic turnover. These enzymes catalyze the breakdown of complex pollutants, frequently by electron shuttling, radical-mediated routes, or cofactor-assisted transformations. Through kinetic modeling, spectroscopic research, and computer simulations, a deeper mechanistic knowledge of these enzymatic systems has been developed, providing insight into structure-function correlations, rate-determining stages, and reaction intermediates. There is potential for next-generation, sustainable pollution remediation technologies that can handle challenging environmental issues by combining these various catalytic approaches (Yentekakis *et al.*, 2020).

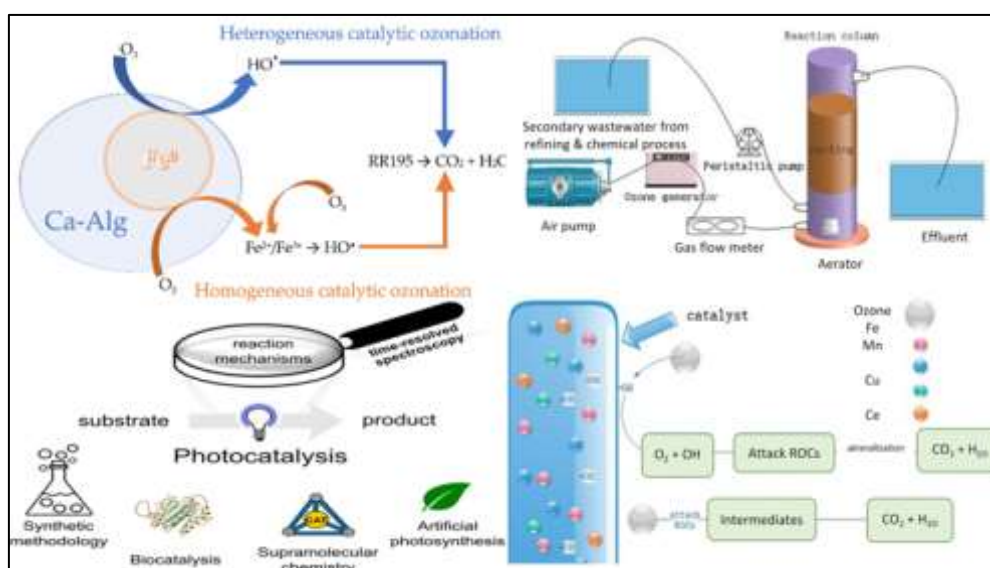


Fig. 1: Catalytic Pathways for Pollutant Removal

Emerging Contaminant Behavior

In environmental and engineered treatment systems, emerging contaminants, including microplastics, endocrine-disrupting chemicals (EDCs), and engineered nanomaterials, behave in complicated and frequently unanticipated ways (Shanmuganathan *et al.*, 2023). This behavior is mostly controlled by the molecular-level interactions that these pollutants have with treatment media. Microplastics easily absorb heavy metals and persistent organic pollutants because of their huge surface area and hydrophobic nature, which complicates traditional removal procedures and creates a dynamic vector for contamination movement. As a result of biofouling and environmental aging, their surface chemistry changes with time, changing their reactivity with membranes and adsorbents in treatment facilities. Because of their structural diversity and capacity to persist at trace concentrations, endocrine-disrupting compounds, which are generally defined by low molecular weight and high polarity, have strong affinities for organic matter, ion-exchange resins, and activated

carbon, but their removal is frequently insufficient (Vieira *et al.*, 2020). The effectiveness of therapy may be further complicated by the possibility that these substances will undergo transformation events, such as oxidation or hydrolysis, that result in equally or more hazardous metabolites. Through processes including electrostatic attraction, van der Waals forces, and hydrogen bonding, nanomaterials, including metal and carbon-based nanostructures, interact with treatment media. However, the behavior of these materials is extremely sensitive to the characteristics of the media, such as pH, ionic strength, and surface charge. Both positive outcomes, like improved pollutant breakdown, and negative outcomes, such as bioaccumulation or catalyst poisoning, can result from their high reactivity and mobility. Designing cutting-edge treatment systems that can effectively target and eliminate such complex pollutants while reducing the production of hazardous transformation products and guaranteeing long-term environmental protection requires an understanding of these molecular interactions (Sharma *et al.*, 2024).

Table 1: Molecular-Level Interactions of Emerging Contaminants with Treatment Media

Emerging Contaminant	Type/Subclass	Treatment Media	Interaction Mechanism	Molecular-Level Processes	Effect on Treatment Efficacy	Research Trends & Notes
Microplastics (MPs)	Polyethylene, polystyrene, PET, PVC	Activated carbon (AC)	Physical adsorption and van der Waals interactions	π - π stacking (for aromatic MPs), hydrophobic bonding, surface entrapment	Moderate efficacy; surface fouling of AC possible	New surface-modified AC is being developed for enhanced MP capture
		Biofilm carriers (e.g., MBBR media)	Biofilm entrapment, surface roughness entrapment	Electrostatic interactions, weak hydrogen bonding	Biofilms can degrade some co-contaminants but may not alter MPs	Biofilm properties are being engineered for dual MP & EDC capture
		Membranes (UF, NF, RO)	Size exclusion, electrostatic repulsion	Molecular sieving, charge-based filtering	High rejection efficiency; fouling is a challenge	Research into anti-fouling membranes using nanomaterials
		Coagulation-flocculation agents (e.g., alum, FeCl ₃)	Bridging, charge neutralization	Ionic strength alteration, aggregation dynamics	Variable removal; depends on MP size and surface charge	Focus on optimizing floc size and density for MP removal
Endocrine-Disrupting Compounds (EDCs)	Bisphenol A, phthalates, estradiol	Activated carbon	Hydrophobic adsorption, pore diffusion	π - π electron donor-acceptor interactions, hydrogen bonding	High adsorption affinity for non-polar EDCs	Nanoporous ACs with tailored pore size being explored
		Enzymatic media (e.g., laccase, peroxidase immobilized substrates)	Enzymatic oxidation	Electron transfer, formation of reactive intermediates	Highly effective at low concentrations	Immobilized enzymes on supports improve stability and reusability
		Photocatalytic surfaces (e.g., TiO ₂ , ZnO)	Photo-induced redox reactions	Formation of hydroxyl radicals,	High degradation rates under UV/visible light	Doping with metals or carbon to

				electron-hole pairs		expand light absorption range
		Biochar	Surface sorption and functional group interactions	Carboxyl, hydroxyl, and phenolic group bonding	Effective but varies with biochar feedstock and activation	Functionalized biochar with enhanced affinity is under development
Nanomaterials	Silver, TiO ₂ , ZnO, graphene oxide	Membranes (nano-enhanced)	Size exclusion, catalytic surface interactions	Surface charge-dependent adsorption, redox activity	High removal of bacteria/organics; may release nanomaterials into effluent	Development of composite membranes that trap NMs post-treatment
		Ion-exchange resins	Surface adsorption, ion displacement	Ligand exchange, electrostatic interactions	Effective for charged NMs; less so for neutral particles	Selective resins being designed for specific NM types
		Constructed wetlands (CW) with engineered substrates	Sedimentation, adsorption to substrate surfaces	Bio-nano interaction, microbial uptake	Limited removal unless substrates are optimized	Enhanced CWs using biochar or Fe-based materials for NM capture
		Advanced oxidation processes (AOPs)	Hydroxyl radical generation, redox reactions	Fenton-like reactions, electron transfer	Can degrade or transform NMs depending on composition	Research into tailoring AOPs to degrade coated or functionalized NMs
Microplastics & EDC Co-exposure	Complex matrix	Activated sludge	Bioaccumulation and trophic transfer within sludge flocs	Co-sorption and altered bioavailability due to MP surface adsorption of EDCs	Synergistic or antagonistic effects on removal	Investigating combined fate modeling in treatment reactors
		Hybrid treatment systems (e.g., ozonation + membrane)	Sequential degradation and capture	Oxidation of EDCs, followed by MP capture	Enhanced removal but energy-intensive	Hybrid system optimization ongoing for lower energy costs
Microplastics & Nanomaterials Interactions	Contaminant complexes	Sedimentation tanks	Aggregation-enhanced settling	Flocculation due to NM bridging of MPs	Improved settling, potential environmental re-release risk	Studies exploring controlled flocculants and NM behavior
		Electrocoagulation systems	Electrostatic aggregation	Redox reactions and charge alteration	High removal efficiency for both types	Sustainable electrodes under development

Molecular Modeling Approaches in Wastewater Treatment

Density Functional Theory (DFT) for Reaction Mechanisms

In computational chemistry, density functional theory (DFT) has emerged as a key tool for examining reaction mechanisms (Sameera *et al.*, 2012). It provides a strong and reasonably priced way to examine the electronic structure and energetics of intricate chemical reactions. DFT is particularly useful in the study of heterogeneous catalysis and environmental remediation

because of its capacity to precisely predict adsorption energies and describe the kind of interactions between reactants and catalyst surfaces. DFT-based benchmark studies have shed important light on the binding affinities of different molecules on metal, metal oxide, and doped surfaces, clarifying how minute variations in electronic structure or surface composition affect reactivity. The prediction ability of DFT in real-world systems is increased by this research, which frequently evaluates theoretical models against experimental data (Raza *et al.*, 2015). Knowledge of the energy barriers and processes

involved in the breakdown of harmful chemicals requires a knowledge of transition states, which DFT has proven crucial in discovering and describing in the context of pollutant degradation. For instance, by identifying important intermediates and activation energies, DFT-based transition state analysis enables researchers to map out the whole reaction cycle of processes like the

photocatalytic degradation of organic pollutants or the catalytic reduction of nitrogen oxides. This mechanistic understanding helps to optimize reaction conditions for maximum efficiency and selectivity in pollution removal procedures, in addition to informing catalyst design (Ahn *et al.*, 2019).

Table 2: Molecular Modeling Approaches in Wastewater Treatment: Applications of Density Functional Theory (DFT)

Approach	Objective	Pollutants Studied	Materials/Surfaces Investigated	Key DFT Parameters	Findings/Outcomes	Implications for Wastewater Treatment
DFT for adsorption energy calculations	Evaluate strength and nature of pollutant binding	Heavy metals (Cd ²⁺ , Pb ²⁺ , Hg ²⁺), organic dyes	Graphene, TiO ₂ , ZnO, activated carbon, MXenes	GGA-PBE, LDA, B3LYP; Cut-off energy: 400–500 eV; k-point mesh: 3x3x1	Adsorption energies ranged from -0.3 eV to -2.8 eV depending on pollutant and material	Insights into suitable adsorbents for pollutant removal based on thermodynamic favorability
DFT-based electronic structure analysis	Determine HOMO-LUMO gap, charge transfer pathways	Antibiotics (ciprofloxacin, tetracycline), EDCs	MoS ₂ , CNTs, Fe-doped graphene	DOS, PDOS, Mulliken charge, Bader charge analysis	Electron transfer promoted by dopants and defect engineering	Enhances photocatalytic and redox reactivity under visible light
DFT for surface reactivity	Elucidate active sites and surface interactions	Phenol, bisphenol-A, formaldehyde	Metal oxides (Fe ₂ O ₃ , CeO ₂), zeolites	Slab models with vacuum spacing, dipole corrections	Reactive adsorption confirmed at oxygen vacancy sites	Suggests surface modification strategies for better degradation
Transition state analysis using DFT	Identify activation barriers and intermediates	Atrazine, paracetamol, nitrobenzene	TiO ₂ , g-C ₃ N ₄ , perovskites	NEB method, frequency analysis, IRC path analysis	Activation energies between 0.8–2.3 eV depending on pollutant	Guides optimization of catalytic conditions (e.g., pH, temperature)
DFT with solvation models (PCM, COSMO)	Simulate aqueous phase interactions	Chlorinated hydrocarbons, arsenate	Functionalized surfaces, polymeric membranes	Implicit solvation models integrated with B3LYP	Water-mediated stabilization of intermediates observed	Enhances reliability of models for real wastewater systems
Benchmarking studies using DFT	Validate adsorption and degradation mechanisms	Multiple (Cr(VI), Pb(II), dyes, antibiotics)	GO, doped metal oxides, biochar models	Comparison with experimental isotherms and spectra	Good correlation with experimental FTIR and adsorption trends	Confirms predictive accuracy and reliability of DFT approaches
DFT for redox potential estimation	Assess oxidation/reduction feasibility	Cyanide, sulfide, azo dyes	Graphene-based materials, TiO ₂ -N co-doped	Gibbs free energy of redox reactions	Predicts spontaneity and electrochemical feasibility	Supports selection of photocatalysts or Fenton agents
DFT-assisted catalyst screening	Identify promising catalytic surfaces	PPCPs (personal care products), NSAIDs	Ni-doped TiO ₂ , Cu ₂ O, AgNPs	d-band center, adsorption energy, charge density maps	Correlation between d-band position and catalytic activity	Accelerates development of new materials for advanced oxidation
DFT for degradation pathway analysis	Map complete degradation steps	Carbamazepine, diclofenac, sulfamethoxazole	TiO ₂ , ZnO, g-C ₃ N ₄ composites	Step-wise energy profile, intermediate structures	Identification of key reactive intermediates (•OH, •O ₂ ⁻)	Helps design systems minimizing toxic intermediate accumulation

DFT for pollutant-metal interaction	Study chelation and complexation effects	Pb ²⁺ , Cd ²⁺ , Cu ²⁺ , Hg ²⁺	Amino-functionalized graphene, EDTA analogs	Ligand field theory, geometry optimization, energy decomposition	Predicts stability constants and coordination geometry	Informs molecular design of chelating agents for heavy metal removal
DFT and machine learning integration	Develop predictive models for adsorption	Broad-spectrum organics and inorganics	Nanomaterials with varied functional groups	DFT-derived features as input for ML (regression, clustering)	High accuracy in predicting adsorption energy trends	Enables high-throughput screening of materials for wastewater cleanup
DFT under varying environmental conditions	Assess temperature, pH, ionic strength effects	Organic pollutants (phenols, nitrophenols)	ZnO, CeO ₂ , Fe ₃ O ₄ composites	Varying dielectric constants, explicit water models	Shifts in adsorption/desorption energies observed	Guides optimization of treatment parameters under real conditions
DFT for degradation synergy studies	Evaluate co-adsorption and competitive degradation	Multi-pollutant systems (e.g., dye + metal)	Dual-functional surfaces (TiO ₂ -Fe ₃ O ₄ , ZnO-CuO)	Energy profiles for sequential and parallel reactions	Demonstrates enhanced or inhibited degradation in binary systems	Supports design of integrated multifunctional catalysts
DFT for membrane fouling prediction	Study interactions between foulants and membrane surfaces	Humic acids, proteins, oils	PES, PVDF, modified membranes	Adsorption site modeling, hydrogen bonding analysis	Identifies fouling hotspots and hydrophobic interaction regions	Aids in antifouling membrane material development
DFT and toxicity prediction	Model transformation products and their toxicity	Pharmaceuticals, pesticides	TiO ₂ , g-C ₃ N ₄ , carbon nitride	Fukui function, electrophilicity index, reactivity descriptors	Some intermediates more reactive/toxic than parent compounds	Provides insight for safer by-product management strategies

Molecular Dynamics (MD) Simulations

A potent computational tool for examining the complex behaviors of atoms and molecules over time, molecular dynamics (MD) simulations offer an in-depth understanding of the dynamics of adsorption and desorption on membranes and nanomaterials (Salahshoori *et al.*, 2024). Through these simulations, scientists can see and measure the molecular interactions between contaminants and artificial surfaces like graphene, metal-organic frameworks (MOFs), carbon nanotubes, and polymeric membranes. MD simulations provide a time-resolved view of how contaminants approach, bind to, or detach from surfaces under various environmental circumstances, making them especially useful for simulating the kinetics and thermodynamics of adsorption processes. MD models can forecast how well materials will capture or release certain pollutants by varying variables like temperature, pressure, surface shape, and chemical functionality. Furthermore, by taking solvent-mediated interactions into account, the addition of explicit solvent models to MD simulations greatly improves their predictive power (Garcia Carcamo *et al.*, 2025). Particularly in watery or complicated environmental systems, solvent molecules are essential for regulating the adsorption energies, diffusion speeds, and orientation of contaminants. By providing insight into solvation dynamics, hydrogen bonding, and hydrophobic interactions, all of which are frequently crucial in adsorption-desorption equilibria, solvent effect

simulations provide a more accurate depiction of pollutant behavior. These simulations speed up the logical design of next-generation nanomaterials and membrane systems for environmental remediation, pollution monitoring, and water purification technologies, in addition to bridging the gap between theoretical modeling and practical data (Zeng *et al.*, 2021).

Multiscale Modeling Techniques

When simulating complex systems, multiscale modeling approaches are essential for bridging the gap between microscopic and macroscopic viewpoints (Wang *et al.*, 2024). This allows researchers to examine phenomena that span wildly disparate time and length scales. The coupling of quantum mechanics/molecular mechanics (QM/MM) is a well-known method in this paradigm that combines the computing efficiency of classical molecular mechanics with the great precision of quantum mechanical computations. In the fields of materials science, biological systems, and catalysis, where electronic effects are confined (such as at a reactive site) yet impacted by a larger molecular environment, this hybrid approach is very useful. The region of interest may be treated quantumly through the use of QM/MM. Such as a catalytic core or the active region of an enzyme, while simulating the nearby atoms using classical mechanics, which requires less computing power, to preserve a balance between

accuracy and scalability (Warshel *et al.*, 2014). Computational fluid dynamics (CFD), which works at the macroscale to represent fluid flow, heat transfer, mass transport, and chemical reactions inside complex systems, such as chemical reactors or biological tissues, is a useful adjunct to such microscale simulation. By offering insights into turbulence, mixing patterns, and residence time distribution, CFD techniques are essential for planning and improving reactor designs. They also solve the Navier-Stokes equations. When combined, QM/MM and CFD offer a thorough multiscale modeling method that covers everything from electronic interactions to reactor-scale phenomena. This enables the entire design and study of industrial processes, innovative materials, and medicines (Nandakumar *et al.*, 2022).

Machine Learning Integration

Predictive modeling for material design and pollutant removal efficiency has been transformed by the incorporation of machine learning (ML) into environmental engineering and materials science, providing a paradigm change from trial-and-error techniques to data-driven innovation (Zhong *et al.*, 2021). By revealing intricate, non-linear correlations between structural characteristics and functional performance, machine learning (ML) facilitates the quick screening and optimization of materials using sophisticated algorithms and data analytics. Using training data from computational simulations and experimental databases, supervised learning models such as random forests, support vector machines, and neural networks are widely used in material design to forecast the stability, reactivity, and physicochemical characteristics of novel materials. ML helps predict the adsorption capabilities, regeneration potentials, and selectivity of materials, including metal-organic frameworks (MOFs), activated carbon, and new nanocomposites under a variety of environmental circumstances, especially in the pollution removal industry (Sharmila *et al.*, 2024). The revolutionary impact of ML-guided material screening is demonstrated by case studies. For instance, researchers have used ML models to quickly and accurately sort through thousands of hypothetical MOFs to find the best candidates for CO₂ capture and heavy metal adsorption. Similar to this, deep learning frameworks have been utilized to significantly shorten development times by predicting the best synthesis pathways for photocatalysts used in wastewater treatment. ML continues to close gaps in material discovery and application as computing power and dataset accessibility increase, spurring sustainable solutions in pollution abatement (Kumari *et al.*, 2024).

Material Design for Advanced Wastewater Treatment

Design of Adsorbents and Catalysts

With the creation of metal-organic frameworks (MOFs), covalent organic frameworks (COFs), nanocomposites, and bioinspired materials, all of which

are optimized computationally for improved performance, the design of sophisticated adsorbents and catalysts has seen tremendous progress (Jaid *et al.*, 2024). Because of their large surface areas, adjustable porosity, and variety of uses, metal-organic frameworks (MOFs), which are made up of metal ions coupled to organic ligands, are perfect for selective adsorption and catalysis, including gas separation, CO₂ capture, and photocatalytic processes. The modular architecture and exceptional thermal stability of COFs, wholly organic crystalline porous materials, allow for fine structural control and functional group integration for particular catalytic pathways or pollutant adsorption. By combining nanoparticles with matrices such as carbon-based materials or polymers, nanocomposites work in concert to provide multipurpose platforms with enhanced reactive surface sites, mechanical strength, and chemical resistance. Because of their improved electron transport capabilities and customized interface features, these composites are particularly useful in environmental remediation and heterogeneous catalysis (Wang *et al.*, 2022). By providing specificity and sustainability, bioinspired materials, which are frequently created using green synthesis methods, bring a fresh perspective to the design of adsorbents and catalysts by imitating natural enzymes or structures. Crucially, the rational design of these materials now heavily relies on computational tools like density functional theory (DFT), machine learning, and molecular dynamics simulations, which allow the prediction and optimization of structural and functional properties before experimental synthesis. The development of high-performance adsorbents and catalysts is accelerated by this combination of computational design and improved materials, providing potential answers in domains such as green chemistry, environmental research, and energy (Dell'Angelo *et al.*, 2022).

Membrane Materials

Membrane materials are essential to contemporary separation technologies, especially for gas separation, water treatment, and biological applications (Iulianelli *et al.*, 2020). Deep insights into the molecular-level interactions governing membrane performance, particularly concerning fouling resistance and selectivity, have been made possible by recent developments in computer modeling. A major obstacle to membrane function is fouling, which is brought on by the buildup of organic materials, microbes, or other particles and frequently results in decreased permeability and a shorter membrane lifespan. Researchers can now anticipate the atomic-scale interactions between different membrane materials and solvents, and foulants, thanks to computational methods like density functional theory (DFT) and molecular dynamics (MD) simulations. With the use of these insights, membrane surfaces may be logically designed with specific hydrophilicity, surface charge, and roughness to reduce foulant adherence and improve cleaning effectiveness (Al-Amoudi *et al.*, 2007). By simultaneously discovering structural motifs

and functional groups that promote certain solute-solvent interactions, computational screening speeds up the tuning of selectivity. This has made it possible to create hybrid membranes that combine the advantages of metal-organic frameworks (MOFs), polymers, and inorganic nanoparticles. These hybrid membranes, which are the result of molecular engineering, provide greater selectivity and fouling resistance along with synergistic qualities, including improved mechanical stability, heat resistance, and customizable pore shapes. In the end, the design paradigm for next-generation membranes has been completely transformed by the combination of computational insights and materials science, allowing for more effective, sustainable, and focused separation processes in a variety of sectors (Singh *et al.*, 2025).

Photo-/Electrocatalytic Materials

Materials that are photo-electro-catalytic have become essential for developing environmentally friendly energy and cleanup solutions (Rani *et al.*, 2020). Water splitting, CO₂ reduction, and wastewater treatment are made possible by these materials' ability to facilitate redox reactions when exposed to light (photocatalysis) or electricity (electrocatalysis). Adjusting the band structure of photocatalytic materials to maximize light absorption, charge carrier separation, and surface reaction kinetics is essential to increasing their effectiveness. By altering the electronic structure of semiconductors through techniques like elemental doping, heterojunction construction, and defect introduction, band gap engineering increases the visible region of light absorption and facilitates more efficient electron-hole pair generation and migration. By lowering recombination losses and raising quantum efficiency, this fine-tuning directly increases photocatalytic activity. At the same time, energy-efficient treatment procedures like electrochemical oxidation of contaminants or electro-Fenton reactions depend equally on the sensible design of electrocatalysts. To reduce overpotentials and enhance selectivity and durability, electrocatalyst design strategies include modifying the surface morphology, improving the active sites, and incorporating conductive supports (Huang *et al.*, 2017). High surface area and a large number of catalytic sites are features of advanced nanostructured electrocatalysts, such as oxides, sulfides, and single-atom catalysts based on transition metals, which speed up reaction rates and electron transfer kinetics. To further improve treatment efficacy while reducing energy consumption, the synergistic coupling of photo-electrocatalytic capabilities in hybrid systems is also being investigated. This represents a frontier in material innovation for clean energy and environmental applications (Blay *et al.*, 2020).

Green and Sustainable Material Approaches

The future of architecture, product design, and manufacturing is being completely transformed by green and sustainable material techniques that prioritize resource efficiency and environmental responsibility (Dixit *et al.*, 2023). Bio-based materials, which come

from renewable biological resources such as plant fibers, algae, fungi, agricultural leftovers, and biopolymers, are at the front of this revolution. In addition to lowering reliance on fossil fuels, these materials frequently have smaller carbon footprints, are less poisonous, and are biodegradable. The creation of bioplastics, hempcrete, mycelium-based composites, and cellulose nanoparticles is an example of innovations in this field; each has special qualities for structural and functional uses (Voutetaki *et al.*, 2024). These resources are complemented by computational techniques, which are essential for creating and refining environmentally friendly substitutes. Even before a product is physically made, researchers and engineers may forecast material performance, evaluate environmental implications, and cut waste with techniques like life cycle assessment (LCA), finite element modeling, and multi-objective optimization algorithms. To find novel green materials and speed up material selection procedures that strike a balance between sustainability and performance, advanced machine learning algorithms are also being used. Green and sustainable material techniques provide a holistic route toward circular economies, less environmental load, and a more resilient future for materials science by fusing bio-based innovation with computer accuracy (Bin Abu Sofian *et al.*, 2024).

Case Studies and Applications

Computational chemistry case studies have shown impressive results in speeding up the development of materials for wastewater treatment, bridging the gap between theoretical predictions and real-world applications (Sandoval-Pauker *et al.*, 2023). The development of metal-organic frameworks (MOFs) for heavy metal adsorption is one such example. Specific MOF structures with high binding affinities for lead and cadmium ions were found by computational simulations employing density functional theory (DFT). These structures were subsequently synthesized and physically verified to have higher adsorption capabilities, hence verifying the prediction models. Similarly, time-dependent DFT was used to predict the best dopant elements and configurations that improve visible-light absorption in the creation of photocatalysts such as doped TiO₂ for degrading pharmaceutical pollutants. Laboratory synthesis and testing later confirmed these theoretical predictions, demonstrating improved photocatalytic degradation efficiency in actual wastewater settings (Frontistis *et al.*, 2012). In another instance, researchers were able to fine-tune surface functionalization for better adsorption by modeling the interaction of dye molecules with graphene oxide surfaces using molecular dynamics simulations. Strong similarities between computational predictions and experimental results were often found by comparative performance assessments, frequently with deviations of less than 10% in adsorption efficiency or degradation rate. These case studies highlight the importance of computational chemistry in directing resource-efficient, high-impact innovation in wastewater treatment systems

as well as in minimizing trial-and-error in materials discovery (Freese *et al.*, 2024).

Challenges, Limitations, and Future Directions

Despite tremendous progress, there are still substantial obstacles and restrictions that prevent computational modeling in chemistry and material science from being widely applied in the real world (Wang *et al.*, 2019). Scalability is one of the main drawbacks; many high-fidelity models need enormous amounts of computing power, which makes simulating huge or complicated systems, like complete biological beings or intricate industrial processes, difficult. Furthermore, assumptions and simplifications that fail to fully represent the dynamism and variety of real-world settings might impair simulation accuracy. This restriction frequently leads to models that, although sound in theory, may not be as reliable predictors in real-world scenarios. It is nevertheless difficult to bridge the gap between these theoretical ideas and their practical use in industry, especially when it comes to converting model results into useful process enhancements or treatments. Moreover, the integration of computational insights into industrial operations is hindered by the frequent absence of multidisciplinary collaboration and standardization. Emerging technologies, however, present a bright future (Ivanov *et al.*, 2021). There is a fascinating chance to improve model accuracy, optimize simulations, and lower computer overhead by combining artificial intelligence (AI) and machine learning with computational chemistry. Real-time prediction capabilities, enhanced parameter estimation, and pattern recognition in large datasets are all made possible by AI-driven models. In fields including innovative materials, environmental remediation, and medication discovery, these hybrid techniques have enormous promise for creating next-generation treatment strategies. To overcome present constraints and convert computational advancements into workable, scalable solutions, it will be essential to develop collaborative ecosystems that integrate domain knowledge in chemistry, artificial intelligence, and engineering (Vassiliadis *et al.*, 2024).

CONCLUSION

Overall, the use of computational methods in wastewater treatment has transformed the discipline by improving environmental sustainability, predictability, and efficiency. The design, monitoring, and optimization of treatment processes are greatly enhanced by computer models, such as computational fluid dynamics (CFD), artificial intelligence (AI), and machine learning algorithms, according to key results. With the use of these technologies, complex biological, chemical, and physical interactions within wastewater systems may be accurately simulated, resulting in more informed choices and economical fixes. Notably, hybrid models that combine data-driven insights with mechanistic understanding have demonstrated greater performance in managing large-scale data from sensors and control systems, forecasting treatment results, and adjusting to

real-time fluctuations. The usage of digital twins, cloud computing, and Internet of Things (IoT)-enabled smart treatment plants is growing, according to emerging trends. These technologies enable predictive maintenance and real-time system optimization. Furthermore, by enabling autonomous system control and adaptive reactions to changing environmental circumstances, artificial intelligence (AI) breakthroughs like deep learning and reinforcement learning are predicted to further revolutionize wastewater treatment. As the subject develops, tackling upcoming water quality issues and guaranteeing sustainable resource management in the face of urbanization and climate change will require multidisciplinary cooperation and the integration of computational tools with green technology.

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