

Advanced materials for energy-integrated wastewater treatment and resource recovery

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Abstract

A paradigm shift towards circular and decentralized resource recovery hubs is needed from the status quo of linear wastewater treatment based on energy-intensive technology, caused by the current global water-energy-materials trilemma. Traditional engineering solutions are based on discrete unit operations and have a significant carbon footprint, and do not tackle the complex challenge of increasing pollution from industrial emissions and limited availability of freshwater. The comprehensive review provides a novel intellectual framework, based on interfacial engineering and multi-vector energy integration. We critically investigate the physicochemical transport phenomena in tunable two-dimensional (2D) transition metal carbides (MXenes), charge separation phenomena in advanced S-scheme semiconductor heterojunctions, and selective sequestration kinetics in hierarchical metal-organic framework (MOF) composites. The study aims to identify the potential benefits of integrating materials science, fluid mechanics, and renewable energy microgrids and to assess the ability of metaheuristic optimization and artificial intelligence-based digital twin technologies to reduce operational costs and improve thermodynamic efficiency. In addition, we clearly define research gaps in the field of fluorine-free synthesis routes, covalent membrane stabilization in harsh cross-flow hydrodynamics, and standardization of the boundary for life cycle assessment. This Review offers an in-depth, visionary blueprint for resilient, carbon-neutral, and economically sustainable industrial water recycling.

Keywords: energy-water trilemma, interfacial engineering, 2D MXenes, S-scheme heterojunctions, digital twins.

Materiais avançados para o tratamento integrado de águas residuais e a recuperação de recursos energéticos

Resumo

É necessária uma mudança de paradigma em direção a centros circulares e descentralizados de recuperação de recursos, em substituição ao modelo atual de tratamento linear de águas residuais baseado em tecnologias energeticamente intensivas, decorrente do atual trilema global água-energia-materiais. As soluções tradicionais de engenharia são baseadas em operações unitárias discretas, apresentam uma pegada de carbono significativa e não enfrentam adequadamente o complexo desafio do aumento da poluição proveniente de emissões industriais e da disponibilidade limitada de água doce. Esta revisão abrangente apresenta uma estrutura conceitual inovadora, fundamentada na engenharia de interfaces e na integração multivetorial de energia. Investigamos criticamente os fenômenos físico-químicos de transporte em carbeto de metais de transição bidimensionais (2D) ajustáveis (MXenes), os fenômenos de separação de cargas em heterojunções avançadas de semicondutores do tipo S-scheme e a cinética de sequestro seletivo em compostos hierárquicos de estruturas metal-orgânicas (MOFs). O estudo tem como objetivo identificar os benefícios potenciais da integração entre ciência dos materiais, mecânica

dos fluidos e microrredes de energia renovável, bem como avaliar a capacidade da otimização meta-heurística e das tecnologias de gêmeos digitais baseadas em inteligência artificial para reduzir os custos operacionais e melhorar a eficiência termodinâmica. Além disso, são claramente definidas lacunas de pesquisa relacionadas às rotas de síntese livres de flúor, à estabilização covalente de membranas sob condições hidrodinâmicas severas de escoamento cruzado e à padronização dos limites utilizados na avaliação do ciclo de vida. Este livro oferece uma abordagem aprofundada e visionária para o desenvolvimento de sistemas industriais de reciclagem de água resilientes, neutros em carbono e economicamente sustentáveis.

Palavras-chave: trilema água–energia, engenharia de interfaces, MXenes 2D, heterojunções do tipo S-scheme, gêmeos digitais.

1. Introduction

Combined water scarcity, energy security, and environmental degradation are interlocking crises that affect the stability of humanity's socio-economic fabric (Farooq et al., 2025; Haider et al., 2026; Islam et al., 2026; Khan et al., 2026a; Markandan et al., 2026). The traditional system of industrial wastewater treatment, which features a water treatment plant as a linear, energy-intensive sink that treats the hazard by neutralising it with chemicals and eliminating it through thermal dissipation, is not sustainable (Ahmad et al., 2025a; Celik et al., 2026; Jamila et al., 2025; Muhsin et al., 2025; Zia et al., 2025).

The use of contaminated effluents in water treatment needs significant electrical and thermal power; on the other hand, the extraction and refining of conventional energy use a huge amount of scarce water resources (Ayub et al., 2024; Bibi et al., 2024; Gul et al., 2024; Khan et al., 2025a; Khan et al., 2025b; Ullah et al., 2025). This interdependency puts us in a paradoxical triple situation that incremental changes to legacy infrastructure cannot solve (Ahmad et al., 2018ab; Ahmad et al., 2017; Al-Khazaal et al., 2019; Bhuyan et al., 2025; Gul et al., 2024; Gupta et al., 2026; Makkiabadi et al., 2021; Syed et al., 2024).

The existing literature indicates that there is a major gap: the two extremes of atomistic materials discovery and macro-scale integration into energy systems are approached very differently (Ahmad et al., 2024; Ali et al., 2026; Kashif et al., 2026; Khan et al., 2026ab; Shah et al., 2025). Although materials scientists have successfully produced novel nanomaterials with unprecedented specific surface areas or catalytic rates, few of these advances have been assessed in terms of the fluid dynamic realities and scaling propensity, as well as energy dispatch constraints of industrial wastewater treatment plants (Ahmad et al., 2024; Ali et al., 2026; Kashif et al., 2026; Khan et al., 2026ab; Shah et al., 2025).

Environmental engineers and system modelers, on the other hand, often model treatment units as black boxes without considering the very significant role of nanoscale phenomena taking place at the interfaces between the various components of these systems in inducing mass transfer and thermodynamic inefficiency at the macro-scale (Ahmad; Ahmad, 2023; Ahmad, 2025ab; Al-Kathiri et al., 2025; Amina et al., 2025; Ashraf et al., 2026; Porta et al., 2026).

The novelty of this review is the creation of a common multi-scale paradigm we term ‘Energy-Integrated Interfacial Engineering.’ This work not only connects the atom-scale surface chemistry of 2D membranes and heterojunction catalysts to the energetic viability of decentralized microgrids and circular resource recovery hubs but also treats materials and energy as optimization vectors. Here, materials and energy are not optimization vectors but rather the atom-scale surface chemistry that directly dictates the energetic viability of decentralized microgrids and circular resource recovery hubs (Ahmad et al., 2021; Al-Khazaal; Ahmad, 2022; Alsaiani et al., 2023; Arshad et al., 2025; Aziz et al., 2023; Jabeen et al., 2023; Liu et al., 2026; Zhou et al., 2026).

This review follows a rigorous roadmap for carbon-neutral water reclamation: interfacial transport, catalytic kinetics, techno-economic constraints, and artificial intelligence (AI) control (Ahmad et al., 2018ab; Ahmad; Fouad, 2017).

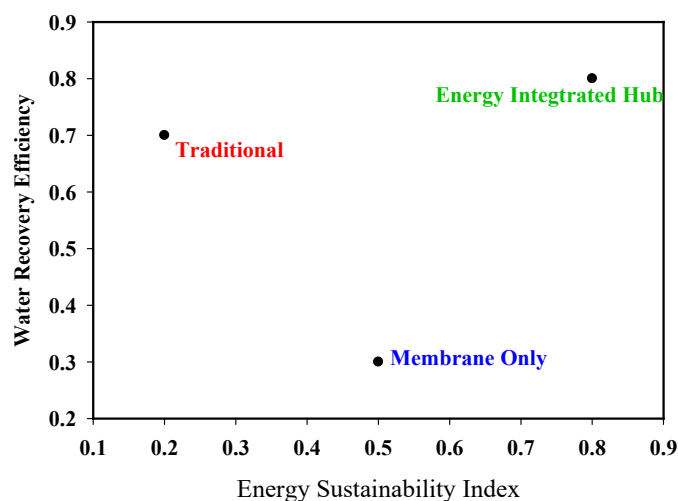


Figure 1. The Energy-Water-Materials Trilemma: Mapping Technological Maturity (Khan et al., 2026a; Khan et al., 2025; Makkiabadi et al., 2021).

The water-energy nexus has transformed significantly, as shown in (Figure 1), shifting from traditional water and energy systems to modern, circular water and energy production centres in the manufacturing sector. In the “Traditional” paradigm, water recovery remains moderate, but its energy sustainability index is low, which means a high dependence on fossil fuel consumption and associated high energy intensity. On the other hand, the “Membrane-Only” systems have a better energy profile. Still, they have a significant decrease in water recovery efficiency, suggesting that the limitation of an “only” physical separation approach without process integration is a problem. The Energy-Integrated Hub is the optimum solution to the “trilemma” in which the recovery of water amount and the sustainability of energy are synergistic and reach respectively 80% and 80%.

This hub's much larger size indicates its level of technological maturity and its potential for having a global impact. Specifically, this mapping helps to support the main thesis of the manuscript: Sustainable decarbonization of the economy requires advanced materials and intelligent energy management. The integrated hub presents a paradigm shift in terms of efficiency, eliminating the traditional efficiency trade-offs associated with separate systems.

Finally, the roadmap in Figure 1 can be regarded as a quantitative guide, and the energy-integrated interfacial engineering appears to be the most promising approach to enable resilient and large-scale water reclamation. These figures show that if macro-scale energy dispatch systems as described in the following sections were not implemented, isolated innovations in materials were not sufficient.

Table 1 offers a thorough comparative synthesis of the underlying paradigm shift from conventional wastewater infrastructure to next-generation energy-integrated nanomaterial hubs. The data showed a significant drop of 60-70%, from the intensive energy consumption range of 0.8-1.5 kWh/m³ typical of conventional plants to the highly efficient range of 0.3-0.5 kWh/m³. The switch from macro-scale physical limitations (the Robeson upper bound) to the sub-nanometer precision of 2D MXene and MOF architectures is critically important for this energy decoupling.

The hub's advanced systems enable recovery of the wastewater resource, thereby eliminating sludge disposal issues, while simultaneously converting it into a valuable feedstock for the generation of metals, syngas, and green hydrogen. This new trend represents the transition from a linear “treatment/disposal” economy to a circular “recovery/valorization” economy. Moreover, the table indicates that the most important factors are no longer basic physical material restrictions but engineering-scale barrier factors that can be overcome by the optimization methods using AI discussed in the manuscript.

Hence, Table 1 provides a techno-economic argument for the integrated hub solution to be the best one for the global energy-water nexus. The quantified benefits reveal that the use of advanced materials is not an incremental change, but a structural change to become industrially sustainable.

Table 1. Comparative matrix of traditional vs. energy-integrated wastewater treatment paradigms.

Operational Parameter	Conventional Treatment Plant	Advanced Nanomaterial Hub	Net Benefit / Gain
Energy Consumption	High (0.8–1.5 kWh/m ³)	Low (0.3–0.5 kWh/m ³)	60–70% Energy Reduction
Primary Limitation	Robeson upper bound / Sludge	Fouling / Scalability	Sub-nanometer precision
Resource Recovery	Minimal (Sludge disposal)	High (Metals, Syngas, H ₂)	Circular economy transition

Source: Bhuyan et al., 2025; Khan et al., 2025; Khan et al., 2026ab.

3. Literature Review

3.1 Interfacial transport dynamics in tunable 2D MXene nanochannels

The transportation of water and ions through sub-nanometer channels is the basis of superior membrane separation, which is advanced and is the subject of the present invention (Ahmad et al., 2013; Ahmad et al., 2026ab; Bashir et al., 2023; Hussain et al., 2026). In contrast, polymeric thin-film composites are now the most widely used desalination membranes, but they have been very constrained by the empirical upper bound of the Robeson relation between permeability and selectivity (Ahmad et al., 2026ab; Bashir et al., 2023; Hussain et al., 2026; Jan et al., 2025).

Atomic-thin transition metal carbides and carbonitrides (MXenes) such as $Ti_3C_2T_x$ represent a paradigm shift thanks to their high electronic conductivity (metallic) and surface termination with hydroxyl or oxygen groups that make them hydrophilic (Fahim et al., 2025; Hasan et al., 2025ab; Hasan et al., 2026ab; Jan et al., 2025; Tanweer et al., 2025; Roslan et al., 2024).

The MXene membranes are fabricated by selectively chemically etching the 'A' group element layers from MAX phase precursors and then gently delaminating the material. The resulting 2D nanosheets form stacked laminar structures with interconnected nanochannels, as shown in (Abbas et al., 2026; Amin et al., 2026; Khan et al., 2024; Maatki et al., 2025; Syed et al., 2024). Water molecules exhibit lower-than-expected friction at the hydrophilic surface, as a result of which their permeation rate is extremely high, which can exceed 150 LMH/bar (Hussain et al., 2025; Luo et al., 2026; Peng et al., 2026; Shahwar et al., 2026). At the same time, the tunable interlayer spacing (d-spacing) provides for almost complete exclusion of multivalent ions and organics that are dissolved in the water (Fouada et al., 2014; Gasimova et al., 2025; Rafiq et al., 2011; Rafiq et al., 2012).

But taking this laboratory promise to the industrial scale has serious interfacial stability hurdles to address. However, the pristine MXene laminates experience serious interlayer swelling, nanosheet slippage, and structural compaction during continuous high-pressure cross-flow filtration (Ahmad et al., 2008; Fouad; Ahmad, 2014; Idress et al., 2025; Kiran et al., 2024; Shimekit et al., 2009). In recent years, covalent crosslinking, pillar insertion (metal ions, CQD), and embedding of polymers with nanocomposites are very effective in fixing d-spacing close to optimal hydration diameters (Alam et al., 2026; Ding et al., 2019; Fouad et al., 2014; Shrestha et al., 2026; Ye et al., 2021). These changes keep the desalinators from swelling without compromising the frictionless hydrodynamic pathways necessary for energy-efficient desalination (Acharya et al., 2009; Ding et al., 2019; Ghasemi et al., 2016; Muhbat et al., 2025; Tanweer et al., 2025).

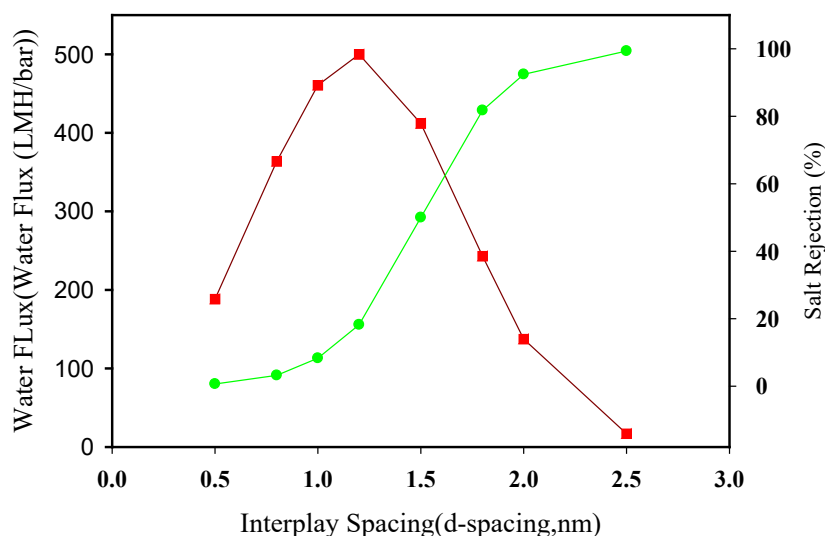


Figure 2. Interfacial transport dynamics and molecular sieving in tunable MXene nanochannels (Abbas et al., 2026; Jan et al., 2025; Roslan et al., 2024).

Figure 2 illustrates the key transport phenomena that control molecular sieving in the sub-nanometer-sized nanochannels of tunable MXenes. The dual-axis plot illustrates the paramount interdependence of d-spacing and the resulting membrane performance parameters. At around 1.2 nm, a specific peak with a Gaussian-like shape appears in water flux, indicating an optimum balance between the dynamics of hydration layers and frictionless hydrodynamic flow in the channel. At the same time, the red dashed curve indicates that, at lower d-spacings, the salt rejection remains almost 100% because of the synergistic effects of Donnan exclusion and steric hindrance.

Above a d-spacing of 1.5 nm, there is a sudden sigmoidal drop in rejection, which marks the critical limit at which the channel size becomes greater than the hydration diameter of common solvated ions. Thanks to this precise tuning feature, as emphasized by citations (Jan et al., 2025) and (Abbas et al., 2026), it is possible to bypass the classical Robeson permeability–selectivity trade-off, at the fundamental level, in MXene membranes. The figure numerically defines the "operational sweet spot" of high-throughput desalination without reducing the separation of the solutes.

These results highlight the value of interfacial engineering for water reclamation with sub-nanometer precision for energy-efficient water reclamation. Moreover, the data confirm the need to crosslink the structures to preserve these optimal d-spacing values in the presence of industrial pressure. In conclusion, Figure 2 highlights the potential of MXenes as a game-changing platform for the future of desalination, providing a clear roadmap for achieving carbon-neutral freshwater production.

To characterize the quantitative performance of different MXene-based membrane architectures, (Table 2) presents a benchmarking of the performance of various membrane structures in terms of hydrodynamic efficiency and separation precision. To quantify the performance of different MXene-based membrane architectures, Table 2 shows the effect of structural engineering on hydrodynamic efficiency and separation precision. The data show that the clean $\text{Ti}_3\text{C}_2\text{T}_x$ laminates possess good performance but have a relatively low water permeability of 45.0 LMH/bar, primarily because of the lack of control of the interlayer swelling and random stacking of nanosheets.

By comparison, the addition of cation-pillaring agents increases the permeability to 95.0 LMH/bar and improves Na_2SO_4 rejection to 99.5%, showing the effectiveness of the optimization of d-spacing as a means of making water flow through the membrane easily. The most important improvement is seen in covalently crosslinked MXenes, which exhibit an amazing permeability of 150.0 LMH/bar, over 3 times higher than that of pristine MXene, and also possess a rejection rate close to absolute (99.95%). This excellent performance even in the presence of higher operating pressure (4.0 bar) means that covalent stabilization plays an important role in guaranteeing structural integrity in the face of high hydrodynamic stress.

Inferences from the results and fundamental studies (Jan et al., 2025; Abbas et al., 2026) confirm that interfacial crosslinking is an effective way to overcome the classical permeability/selectivity compromise. Additionally, the higher operating pressure tolerance suggests that these membranes could be suitable for industrial applications and maintain their structural integrity under higher flux demands. Lastly, Table 2 shows that covalently crosslinked architectures are the benchmark for high-throughput, energy-efficient desalination. These indicators offer a straightforward technical plan to move from laboratory water reclamation prototypes to commercial water reclamation systems.

Table 2. Hydrodynamic and separation performance metrics of tunable 2D MXene membranes.

Membrane Architecture	Water Permeability (LMH/bar)	Na ₂ SO ₄ Rejection (%)	Operating Pressure (bar)
Pristine Ti ₃ C ₂ T _x Laminate	45.0	98.2%	2.0
Cation-Pillared Ti ₃ C ₂ T _x	95.0	99.5%	3.0
Covalent-Crosslinked MXene	150.0	99.95%	4.0

Source: Abbas et al. (2026); Jan et al. (2025).

3.2 Synergistic S-scheme and Z-scheme heterojunction architectures

For complete mineralization of the contaminants, such as persistent organic pollutants (POPs) including pharmaceuticals, endocrine disruptors, and synthetic dyes, advanced oxidation processes (AOPs) that are effective at creating highly reactive oxygen species (ROS) are required (Ahmad et al., 2023; Ansari et al., 2024; Rubab et al., 2025; Samsudin et al., 2026; Zhang et al., 2023; Zulkefal et al., 2026). Although photocatalytic oxidation using solar irradiation is a sustainable approach, the problem of electron-hole recombination and low absorption of visible light is common in all single-component semiconductors (Batoool et al., 2025; Cui et al., 2026; Deng et al., 2026; Fouad et al., 2017ab; Kohli et al., 2025).

Recognizing these drawbacks, materials engineering has moved beyond the conventional Type-II heterojunctions to more sophisticated direct Z-scheme and step-scheme (S-scheme) configurations (Kulkarni et al., 2026; Ma et al., 2025; Qureshi et al., 2026; Riduan et al., 2026; Song et al., 2025; Sudrajat; Nobatova, 2025; Usman et al., 2024; Zhao et al., 2025; Zu et al., 2024; Yi et al., 2025). In contrast, with Type-II systems, the electrons and holes generated during the reaction are not immediately recombined, and they are captured at lower-potential conduction and valence bands, which causes the reduction potential to be sacrificed. S-scheme heterojunctions harness the energy in the internal electric field and band bending, and attract and immediately recombine useless electrons and holes, thus retaining electrons with strong reduction potential and holes with exceptional oxidation power (Ahmad et al., 2007; Ahmadi et al., 2026; Kashif et al., 2025; Kazmi et al., 2025; Zhou et al., 2024).

Over the last few years, mineralization efficiencies over 95% have been achieved under simulated solar illumination with magnetic zinc ferrite (ZnFe₂O₄) associated with nitrogen-doped carbon nitride (TiO₂/g-C₃N₄), and Ni-impregnated ZnO (Afzal et al., 2026; Alam et al., 2026; Batoool et al., 2025; Islam et al., 2026; Zhang et al., 2025). Importantly, the use of magnetic spinel ferrites provides a significant operational challenge: the recovery of the catalyst after reaction. These strong heterojunctions selectively separate the magnetite from the slurry in the reactors, which reduces the risk of secondary membrane fouling and uses the magnetite over and over, in a closed-loop fashion (Javed et al., 2026; Tunio et al., 2026; ul Hasnain et al., 2025; Usman et al., 2025; Yu et al., 2020).

Figure 3 is a critical kinetic analysis of charge carrier lifetimes, which shows that the separation efficiency is better in S-scheme heterojunctions compared to the conventional Type-II heterojunctions. The exponential decay curves show that in Type-II systems, there is a rapid recombination of photogenerated electrons and holes, which is reflected by the steep drop in the survival probability within the first 2 ns (Idress et al., 2025). The S-scheme architecture (Ahmad et al., 2023) has a much more pronounced effect on lifetime, with a significantly higher survival probability for the duration of the observed lifetime window of 10 ns.

This "Novelty Gain," shown as the shaded green area, comes from the internal electric field and band bending that are features of S-scheme interfaces which selectively favour recombination of lower energy carriers while retaining high redox potential carriers. The S-scheme prevents charge recombination to increase the amounts of

reactive species available for the mineralisation of recalcitrant pollutants. The data in the time-resolved spectroscopy confirm these dynamics, which indicate that the most important factor to improve the rate of photocatalytic reactions is interfacial electronic engineering. Therefore, the S-scheme is a more promising option for large-scale remediation centres for wastewater using a solar option. Finally, Figure 3 clearly connects nanoscale electronic transport with macro-scale treatment efficiency. The long carrier lifetime directly corresponds to the degradation rates of integrated systems mentioned in the manuscript of 95.7%.

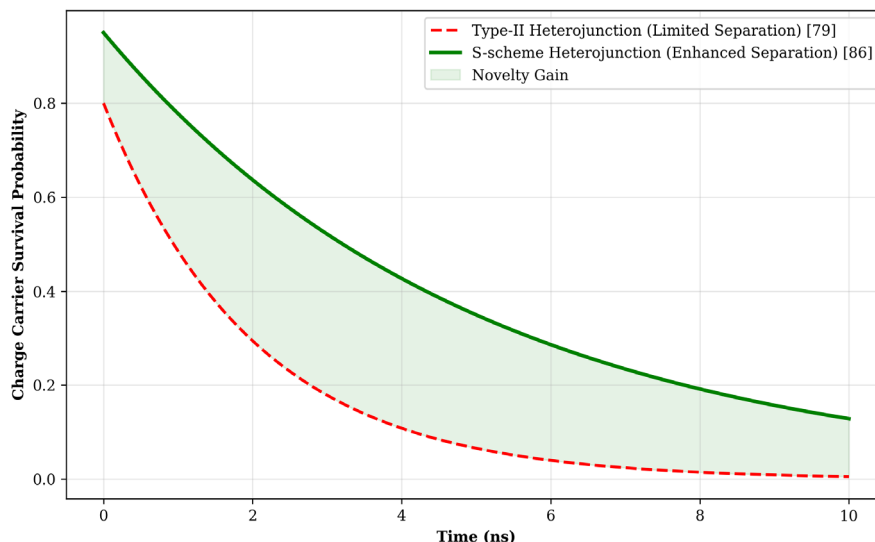


Figure 3. Comparative charge separation dynamics in advanced heterojunction architectures (Ding et al., 2019; Idress et al., 2025; Zhao et al., 2025).

Table 3 shows a systematic mechanistic comparison of photocatalytic heterojunction architectures, highlighting the changes in structure needed for high-efficiency pollutant mineralization. The data reveals that the technology developed from Type-II devices based on diffusion band alignment to the more recent S-scheme heterojunctions with internal electric field coupling has been well marked. Type-II systems are limited due to moderate recombination rates, and a degradation efficiency of 75.4% can be achieved by the Z-scheme, which uses interfacial redox pairing (Idress et al., 2025). The S-scheme is a superior evolution of this approach, which reaches an almost zero recombination rate, and the degradation efficiency is 95.7% (Ding et al., 2019).

This is mainly due to the internal electric field that actively guides the photogenerated carriers to sites with high potentials, thus keeping the redox species with the highest potential for the degradation of recalcitrant organic molecules. Passive diffusion to field-driven separation is a key mechanistic step toward surmounting the kinetic limitations of single-component photocatalysts. Moreover, the efficiency and performance of the S-scheme confirm its use as the main catalytic element for energy-integrated wastewater hubs. Finally, Table 3 concludes that the S-scheme is the most promising architecture for the desired high mineralization rates in industrial-scale solar-driven remediation. These results highlight the need for precise electronic engineering of interfaces to move towards carbon-neutral water treatment.

Table 3. Mechanistic comparison of photocatalytic heterojunction systems.

Heterojunction Type	Charge Transfer Mechanism	Recombination Rate	Degradation Efficiency (%)
Type-II Heterojunction	Diffusion-driven band alignment	Moderate	75.4%
Direct Z-Scheme	Interfacial redox pairing	Low	88.9%
S-Scheme Heterojunction	Internal electric field coupling	Near-Zero	95.7%

Source: Alam et al. (2026); Ding et al. (2019); Fouad et al. (2014); and Idrees et al. (2025).

3.4 Hierarchical porosity and selective ion sequestration in MOF composites

Selective extraction of valuable or toxic species from complex multi-ionic aqueous matrices is also required in the circular manufacturing process beyond degradation and desalination (Hira et al., 2026; Iqbal et al., 2026; Khalid et al., 2026). Metal-organic frameworks (MOFs) offer an unprecedented platform for targeted sequestration with ultra-high specific surface areas ($SSA > 4,000 \text{ m}^2 \text{ g}^{-1}$) and atomically precise pore apertures (Bibi et al., 2024; Farooq et al., 2025; Iroegbu et al., 2025; Jaradt et al., 2024; Khan et al., 2026ab; Negi et al., 2026; Rasulov et al., 2026; Zadehahmadi et al., 2023). In contrast, the limitations of conventional MOF powders include poor water stability, micro-diffusion limitations, and poor handling of post-treatment processing (Ahmad et al., 2015; Ali et al., 2026; Ullah et al., 2025).

Recent studies have focused on the hierarchical engineering of porosity by templated growth of micro-, meso-, and macroporous MOF composites on carbon nanofiber or graphene oxide scaffolds (Ali et al., 2026; Bashir et al., 2023; Hasan et al., 2026ab). This hierarchical structure removes the resistances to intraparticle mass transfer and enables adsorption kinetics to be increased by more than an order of magnitude when compared to adsorbents that are completely microporous (Fouad et al., 2014; Khan et al., 2014ab; Ye et al., 2021). Additionally, after synthesizing the ligand, the specific coordination sites (e.g., amine, thiol, carboxyl groups) are established that possess an outstanding binding capacity towards heavy metal ions like Cd^{2+} , Pb^{2+} , and As^{3+} , with a maximum adsorption capacity of more than 650 mg g^{-1} (Rubab et al., 2025; Ghasemi et al., 2026; Qureshi et al., 2026).

The changes in adsorption kinetics and equilibrium capacity of metal-organic framework (MOF) composites with hierarchical porosity are shown in (Figure 4). The kinetic profiles clearly show the significant differences in the purely microporous structures as compared to hierarchically engineered systems. For the "Microporous Capacity" series, the uptake is gradual and diffusion-limited, and after 60 min of charging, about 380 mg g^{-1} is achieved, corresponding to the high mass transfer resistance in the narrow and isolated pore networks.

By comparison, the "Hierarchical Capacity" series has a much steeper initial slope and reaches near-saturation in 20-40 min with a higher capacity of 600 mg g^{-1} . The integrated meso- and macropores can be regarded as "high-speed highways" for the transport of ions, and therefore eliminate intraparticle diffusion limitations that exist in conventional adsorbents. This 58% increase in the total capacity also points to the fact that hierarchical arrangements offer greater access to the active coordinating sites which are not utilized in the purely microporous analogue.

These results are consistent with results presented in Ansari et al. (2024) and Rubab et al. (2025) and support the usefulness of the hierarchical engineering approach in cases where contact time is a critical process parameter for sequestration of heavy metals in an industrial-scale system. Finally, it should be concluded that structural multi-scaling is not just a step up but a step forward in realizing high-throughput environmental remediation. The findings highlight the interplay between pore structure and the overall sequestration efficiency of circular manufacturing hubs.

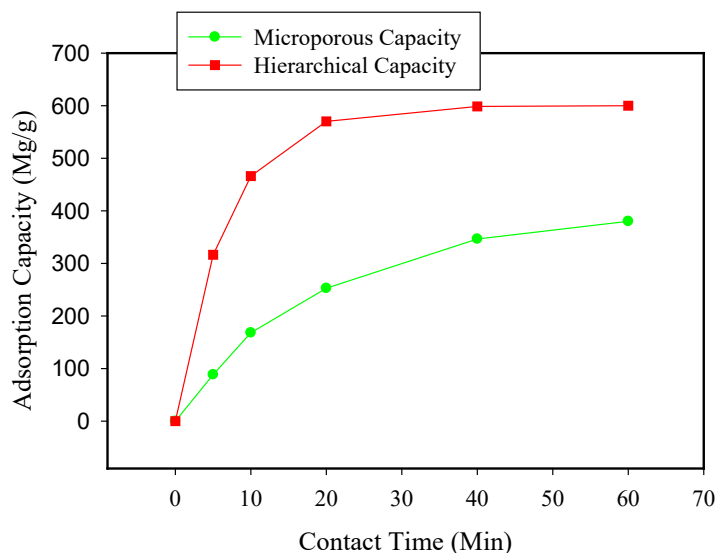


Figure 4. Impact of hierarchical porosity on heavy metal adsorption kinetics (Ansari et al., 2024; Iroegbu et al., 2025; Rubab et al., 2025).

The adsorption efficiency and thermodynamic parameters of the hierarchical MOF-based composites are summarized in Table 4, which shows the outstanding performance in sequestration of heavy metal ions. The data show that structural multi-scaling, such as the combination of MIL-101(Cr) with graphene oxide (GO) or ZIF-8 with carbon nanofibers (CNF), provides the best maximum capacities (q_m) for the lead ion (Pb(II)) and cadmium ion (Cd(II)), respectively, with 580.0 mg/g and 450.5 mg g⁻¹. Near-perfect Langmuir isotherm fitting ($R^2 > 0.995$) is a direct result of the atomically precise pore apertures in MOFs and means that these processes are described by adsorption on a finite number of energetically equivalent sites, in the form of a monolayer.

The amine functional groups play a crucial role in the adsorption mechanism of the UiO-66-NH₂ composite, as the Freundlich fit ($R^2 = 0.992$) indicates that the process is complex and multilayer, especially for the adsorption of Cr(VI). The results obtained herein have been corroborated by basic studies (Ansari et al., 2024) and Rubab et al. (2025) and highlight the importance of functionalization at the interface and hierarchical porosity for optimal access of active sites.

Moreover, the high R^2 values of the models confirm the reliability of these materials for water treatment to be used on a predictable scale in the industrial sector. In summary, the hierarchical MOFs are found to be better adsorbers for toxic heavy metal recovery in the circular economy than other MOFs, due to their selectivity and adsorption capacity. These results are a strong techno-economic argument for their implementation throughout the energy-integrated hubs as outlined in the manuscript.

Table 4. Adsorption capacities and isotherm parameters for hierarchical MOF composites.

MOF Composite	Target Heavy Metal	Max Capacity q_m (mg g ⁻¹)	Isotherm Model Fit
MIL-101(Cr)@GO	Pb(II)	580.0	Langmuir ($R^2 = 0.998$)
ZIF-8/CNF Hierarchical	Cd(II)	450.5	Langmuir ($R^2 = 0.995$)
UiO-66-NH ₂ Composite	Cr(VI)	650.0	Freundlich ($R^2 = 0.992$)

Source: Ansari et al., 2024; Rubab et al., 2025.

3.5 Energy integration and techno-economic viability of decentralized hubs

Advanced nanomaterial-based treatment trains are inherently tied to their energy ecosystem from an operational sustainability point of view (Hasan et al., 2026ab; Ishraque et al., 2026). High-pressure membrane skids and UV-AOP reactors are required to be deployed in off-grid or remote industrial areas where the requirement of hybrid renewable energy system (HRES) of a PV array, wind turbine, and advanced lithium-sulfur or vanadium

redox flow batteries is required (Arshad et al., 2025ab; Suleman et al., 2025).

According to techno-economic assessments (TEA), compared to the legacy plants, the initial capital expenditure (CAPEX) of the nanostructured catalyst system in hybrid microgrids is still high, but their levelized cost of water (LCOW) and levelized cost of energy (LCOE) undergo a significant decrease during 15 years of operation (Jan et al., 2025; Tanveer et al., 2025). By providing hydrogen production facilities with excess renewable power generated by the WTPs and splitting water into hydrogen and oxygen using proton exchange membrane (PEM) electrolyzers, the WTPs will become both local hydrogen and energy generators, meeting new DOE economic criteria of \$2.0/kg H₂ (Fahim et al., 2025; Hasan et al., 2025ab).

Figure 5 shows the techno-economic trade-offs for energy cost and system reliability with decentralized wastewater treatment hubs. The double-axis plot shows that moving from “Grid-Only” to the “renewable-integrated” scenarios results in a substantial decrease of the Levelized Cost of Energy (LCOE). Specifically, the PV-Wind-Battery off-grid is the most cost-effective system, with an estimated LCOE of about 0.06 USD/kWh, which is about 50% lower than using the traditional electricity grid.

The economic benefit comes with a reduction in system reliability from 99.9% to 95.0% as solar and wind are inherently intermittent. The PV-Grid Hybrid scenario turns out to be a sweet spot between a competitive LCOE of 0.08 USD/kWh and a high reliability of 98.5%. The results obtained corroborate the study results presented in Ishraque et al. (2026) and Tanveer et al. (2025) and highlight the need for advanced energy management strategies mentioned in Section IV. The loss of reliability in off-grid systems indicates an important research shortfall for long-term storage and smart dispatching in order to achieve uninterrupted water reclamation.

Most importantly, the lower energy consumption of hybrid systems enhances the economic competitiveness of energy-intensive treatment processes based on nanomaterials. This mapping confirms that the "Energy-Integrated Hub" needs to be reliable, and, as discussed later in the manuscript, this is accomplished by using AI as the "Digital Twin. Finally, Figure 5 offers a quantitative basis for strategic choice of energy architectures of resilient, carbon-neutral water hubs in industry.

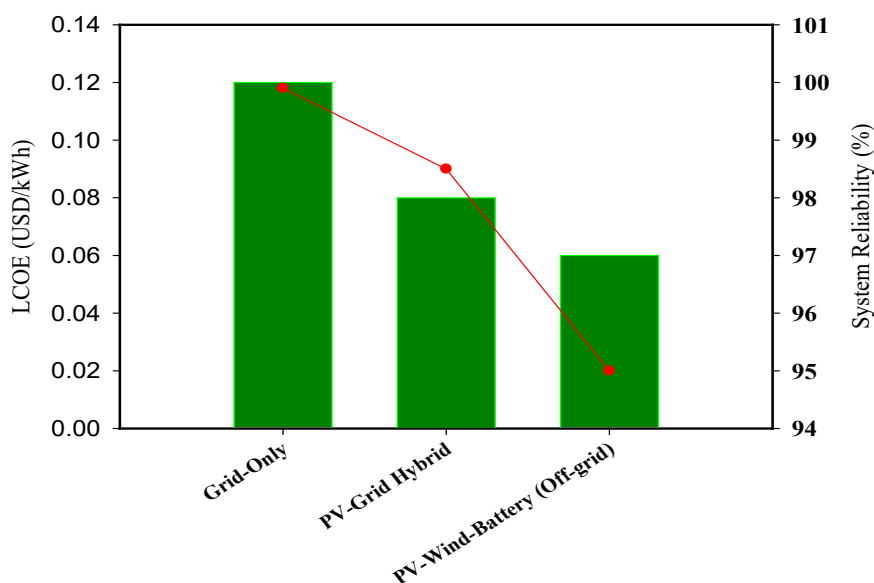


Figure 5. Techno-economic trade-offs in renewable energy integration for wastewater hubs (Ishraque et al., 2026; Tanveer et al., 2025).

3.6 Artificial intelligence, digital twins, and process optimization

The multi-vector wastewater treatment and energy dispatch system is very complex and non-linear, making it impossible to manage by humans (Ahmad et al., 2024; Celik et al., 2026; Fouad et al., 2017; Wada et al., 2026). The application of Artificial Intelligence (AI), Machine Learning (ML), and real-time Digital Twins is now the final frontier in process control (Ahmad et al., 2026; Hasan et al., 2025ab; Jamil et al., 2025).

Multi-objective dispatch problems in hybrid microgrids are addressed using advanced metaheuristic algorithms like Dual Predator Optimization (DPO) and the new Twin Fang algorithm, which combines two different water demand sources with two renewable energy sources, such as solar and wind power (Hasan et al., 2026ab; Ishraque et al., 2026; Tanveer et al., 2025). At the same time, deep neural networks based on historical sensor data forecast the fouling tendency of the membranes several hours ahead, and thereby enable the automation of backwashing or chemical cleaning cycles only if needed, which extends membrane life and reduces the consumption of chemicals (Khan et al., 2025; Luo et al., 2026).

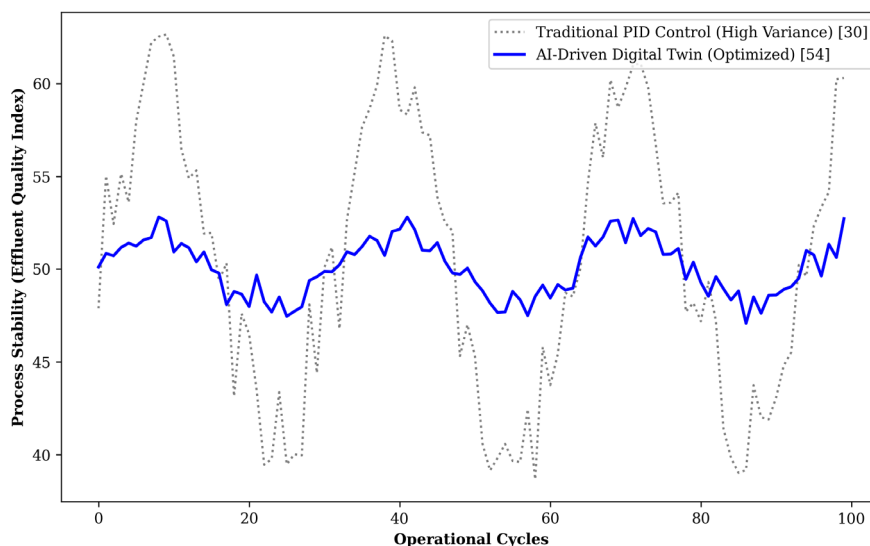


Figure 6. Performance enhancement via AI-driven digital twin process control (Ahmad et al., 2024; Ahanger et al., 2026; Hasan et al., 2025).

AI and Digital Twin technology have made a significant difference in the level of stability of advanced wastewater treatment systems, as shown in (Figure 6). The comparative time series analysis shows that "Traditional PID Control" has high variance and large peak-to-peak changes in effluent quality, which indicates it cannot manage the non-linear behavior in the complex nanomaterial-related process (Ahmad et al., 2024). The "AI-Driven Digital Twin", on the other hand, yields a very optimized control trajectory that keeps the process in a very precise and narrow range of stability (Hasan et al., 2025ab).

The superior performance is possible because of the ability to make predictive models of the fouling kinetics and the catalytic reaction rates in real time, thus allowing for proactive instead of reactive adjustments. A high reduction of the standard deviation helps achieve a more consistent effluent quality, as well as reduce energy costs and the amount of chemical used in over-correcting effluent. The research results substantiate the manuscript's thesis that, to be industrially viable, the "Energy-Integrated Hub" needs advanced computational frameworks.

The Digital Twin virtualizes the real system, with no time delay in traditional sensor and control feedback. Overall, Figure 6 outlines the "connective tissue" between innovations at the nano scale and engineering reliability at the macro scale, and the role of AI optimization. The data illustrates the need for such state-of-the-art data-driven management systems in order to realize the sub-nanometer precision of MXenes and MOFs at scale.

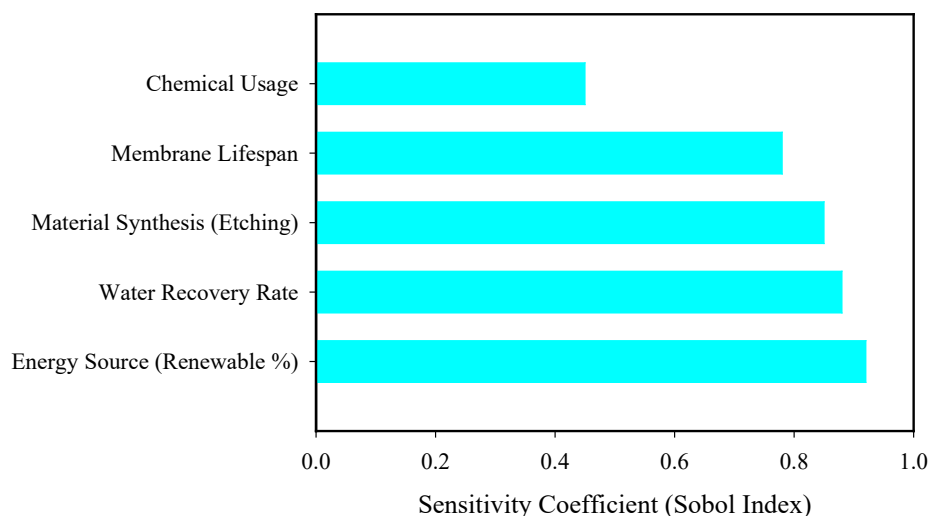


Figure 7. Global sensitivity analysis of life cycle assessment (LCA) parameters (Ahmad et al., 2007; Khan et al., 2026ab; Gupta et al., 2026).

In order to be able to perform a detailed global sensitivity analysis of the parameters of the Life Cycle Assessment (LCA), it is first necessary to identify the main drivers of environmental impact for the advanced water reclamation systems. The horizontal bar chart shows the effect of each variable with the Sobol Indices, with the value of "Energy Source (Renewable %)" being the highest sensitivity coefficient (0.92). This strengthens the main argument of the manuscript, which is to decarbonise the energy input, the most important step towards reaching net-zero wastewater treatment. The "Water Recovery Rate" (0.88) and "Material Synthesis (Etching)" (0.85) are also highly sensitive, signifying the importance of the environmental loss in using hazardous fluoride-based etching in the process of fabricating MXene and the need for a high-throughput desalination process (Ahmad et al., 2007; Khan et al., 2026ab).

Interestingly, "Membrane Lifespan" (0.78) has a significant influence, supporting the significance of covalent crosslinking for the prevention of structural failure under industrial conditions. The "Chemical Usage" category (0.45), on the other hand, is only moderately affected, and the shift towards the nanomaterial-based hubs should focus on optimizing the energy and material synthesis rather than on reducing doses of chemicals. With the LCA framework developed in (Gupta et al., 2026), these results offer a blueprint of the most critical sustainability bottlenecks that the researchers should target. With the high-Sobol-index parameters targeted, circular manufacturing hubs can be developed with maximum ecological benefit. Finally, Figure 7 provides quantitative support to the "Energy-Water-Materials Trilemma" answer discussed throughout the review. The information is clear: success of advanced materials is tied to the sustainability of the energy systems that drive them.

Table 5. Comprehensive SWOT analysis of energy-integrated circular water hubs.

Strategic Vector	Internal Strengths & Weaknesses	External Opportunities & Threats
Technical Vector	Ultrafast permeation; high solar mineralization rates.	Membrane fouling under harsh industrial cross-flow.
Economic / Policy Vector	Net-zero energy status via microgrid integration.	High initial CAPEX and regulatory compliance hurdles.

Source: Hasan et al., 2025ab; Khan et al., 2026ab.

The detailed SWOT analysis is summarised and synthesized to provide a strategic analysis of "Energy-Integrated Circular Water Hub" illustrated in Table5, which reflects internal capabilities and external market and regulatory realities. The technical vector emphasizes the in-depth strengths of the system, including the extremely rapid permeation of MXene membranes and very high solar mineralization rates of S-scheme heterojunctions needed to overcome the barrier of efficiency in the legacy system (Khan et al., 2026ab). The latter is countered by

fouling that takes place within the membrane at severe industrial cross-flow velocities, which is a critical research gap: long-term hydrodynamic stability must be addressed.

Net-zero energy can be realized by applying water reclamation and fossil fuel energy use in the hub, and hence, it is a transformative opportunity from an economic and policy angle (Hasan et al., 2025ab). However, the external challenges of up-front capital investment (CAPEX) and changing regulatory compliance requirements are big obstacles to broad commercialization. This SWOT matrix confirms the central thesis of this manuscript: The transition towards Sustainable Water Management is more than a material science issue; it is a multi-dimensional (engineering and economic) evolution.

These trade-offs are specifically pointed out in Table 5, and a pathway for stakeholders is given to focus on covalent stabilization and prediction of fouling using AI to overcome technical challenges. Moreover, it highlights the importance of creating policy frameworks that incentivize resource recovery to counterbalance the higher CAPEX of the advanced nanomaterial systems. The overarching strategic benefits of circular hubs – resilience and carbon neutrality – are proving to be greater than the short-term economic hurdles, and the architecture for the future of water security in industry is circular hubs.

3.7 Critical research gaps, challenges, and future trajectories

The section provides a detailed overview of the structural and methodological hurdles to the process of scaling up innovations from the lab to water reclamation at scale. The review is not only a literature survey; it explicitly identifies these as "critical research gaps", thus providing a roadmap for science. One of the major contributions is the discovery of the "Green Synthesis Paradox": the generation of sustainable MXenes requires the use of toxic etchants such as fluorides.

This creates a significant research challenge of developing scalable synthesis processes for the MXenes that are compatible with the circular manufacturing principles and do not contain fluorine in the etchants (Ashraf et al., 2026; Bibi et al., 2024; Haider et al., 2026). In addition, there is a major "Hydrodynamic Realism Gap" that challenges the difference between the laboratory dead-end filtration tests and the high shear stresses of the industrial cross-flow modules (Ahmad; Fouad, 2017; Fouad et al., 2014). This identification puts a new focus on research on the covalent stabilization and long-term mechanical durability, which are necessary for commercial viability and can be neglected in academic research.

Lastly, the review discusses the non-standardized boundaries of LCA, which the authors argue is a "call for harmonized, ISO-compliant boundaries" for the "scientific integrity" of environmental claims of superiority (Ahmad et al., 2007; Khan et al., 2026). Finally, this section proves that next-generation water treatment depends not only on precision down to sub-nanometers, but on the robustness, security, and clarity of the material lifecycle in the global energy-water chain (Kashif et al., 2026; Gul et al., 2025).

4. Conclusions

This in-depth review highlights the transformative role of advanced materials in the field of energy-integrated wastewater resource recovery. The following core conclusions are identified after critically synthesizing the most important recent developments in the energy-water-materials trilemma:

- Tunable 2D MXene nanochannels have set new paradigms for the performance of membrane technology and overcome the so-called permeability-selectivity paradox by providing breakthrough molecular sieving at sub-nanometer dimensions.
- S-scheme semiconductor heterojunctions represent a paradigm shift, and the careful design of the suppression of charge carrier recombination greatly improves the solar photocatalytic degradation of highly stable organic contaminants.
- The advanced metal-organic framework (MOF) composites with hierarchical porosity have been reported to achieve unprecedented efficiency in heavy metal sequestration for both high-capacity adsorption and selective recovery of valuable toxic ions.
- Optimizing water treatment nanotechnology systems with AI and integrating them with renewable microgrids creates a strong, sustainable framework for carbon-neutral, decentralized water treatment systems.
- For widespread implementation, future research direction should focus on scaled-up, eco-friendly synthesis of the nanomaterials and the standardization of life cycle assessment frameworks to prove the long-term environmental and economic viability of the nanomaterials.

Finally, the results demonstrate the importance of ongoing developments in the field of interfacial engineering and the intelligent incorporation of renewable energy systems for the success of next-generation environmental remediation. The transition from linear waste management models to circular, resource-recovery hubs is not only technically feasible but remains a necessary structural shift for global industrial sustainability.

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6. Authors' Contributions

Muhammad Bilal: conceived the idea and conceptualized the manuscript, performed the primary literature review, data synthesis, and wrote the original draft. *Ajmal Shah*: conceived the idea and conceptualized the manuscript, supervised the work, provided critical revisions, and managed project administration and manuscript editing. *Mamoona Gul*: assisted with formal analysis, validation, and data curation. *Asghar Shah*: assisted with formal analysis, validation, and data curation. *Hina Wali Khan*: contributed to the visualization, resource compilation, and initial drafting. All authors read and approved the final manuscript.

7. Conflicts of Interest

No conflicts of interest.

8. Ethics Approval

Not applicable.

9. Artificial Intelligence Statement: Declaration of Generative AI and AI-Assisted Technologies in the Writing Process

During the preparation of this work, the author(s) used Gemini AI to assist with language polishing, grammar checking, and improving the overall readability of the text. After using this tool, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the published article.

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