

## Advanced Interfacial Engineering of Hybrid 2D Nanomaterials for Next-Generation Environmental Remediation and Energy Conversion Systems

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### ABSTRACT

The global move towards a low carbon and sustainable economy rests on the basis of advanced materials that are able to overcome the inherent limitations of the current catalytic materials and membranes. This review aims to systematically and comprehensively evaluate the interfacial engineering strategies of hybrid 2D nanomaterials with particular emphasis on the fundamental charge-transfer dynamics and electronic interactions at the heterojunction interface. The manuscript critically summarizes recent progress in MXenes, metal-organic frameworks (MOFs) and semiconductor heterostructures, and explains the exact physical mechanisms behind spatial electron-hole separation, sub-nanometer ionic transport and enhanced surface reaction rate for these systems. The study also examines their application in energy-integrated environmental remediation hubs and the essential role of AI and digital twin technologies in ensuring the integrated system performs effectively at various scales. In addition, critical research gaps, such as the need for scalable, fluorine-free green synthesis methods, and the need for long-term hydrodynamic stability under industrial cross-flow conditions are addressed rigorously. In conclusion, this review provides a solid scientific basis and pathway for researchers and policymakers to tap into the potential of interfacial physics for the resilient implementation of circular bio economies.

**Keywords:** Interfacial Engineering, 2D Nanomaterials, Charge-Transfer Dynamics, MXene-MOF Hybrids, Environmental Remediation, Energy Conversion.

## Introduction: The Imperative for Interfacial Innovation

A transition is needed from linear water-energy-materials approaches to circular resource-recovery centers around the world [1]. The Robeson upper bound has been a challenge in membrane separation and high charge recombination rate in photocatalysis for conventional environmental technologies [2, 3]. The materials with high specific surface area and tunable electronic properties, such as Advanced 2D nanomaterials, including MXenes and MOF-based hybrids, have become new platforms that can significantly change the world [4, 5]. The real power of these materials, however, can be realized through engineered interfaces that enable ultrafast charge transfer and molecular sieving [6, 7]. The urgency of the industrial need for high efficiency and energy integration of wastewater treatment systems to recover valuable resources, such as green hydrogen and syngas [8, 9] has been the driver for this review.

## Research Gaps, Demand, and the Need for this Review

Although a lot of progress has been made, the fundamental translation between lab and industry is still missing [10, 11]. The majority of the available reviews focus on the treatment type, and do not consider the fundamental physics of the interface which governs the performance in different applications [12, 13]. Advanced materials must meet green chemistry principles [14, 15] and there is an urgent need to harmonize synthesis protocols with life cycle assessment (LCA) boundaries to ensure that advanced materials do not violate green chemistry principles. Moreover, there is no standard testing under extreme cross-flow conditions of the industry, which makes the commercialization of 2D laminates difficult [16, 17]. This review aims to fill these gaps by offering a causal structure-interface-mode-signal-reliability framework and understanding reported sensitivities with real-world deployment conditions [18-20].

Table 1 offers a much-needed comparison and synthesis of the interfacial performance of various 2D hybrid architectures, showcasing the profound transformation of remediation efficiency in the era of advanced engineering. Although with such intensity, pristine MXene is limited by surface group modulation, thus with moderate charge transfer rate and efficiency of 85.4%. Optimizing the electronic interface with MXene-MOF heterojunctions (through a Schottky barrier) has been a huge step forward, with efficiencies reaching 94.8%! But the S-scheme hybrid architecture is the better choice, with the charge transfer rate reaching 'ultrafast' and remediation efficiency the best recorded of 98.2%. This leap in performance is achieved by the build-up of a sufficiently strong internal electric field (IEF) that allows for charge separation in space inside the semiconductor while reducing carrier recombination losses. These data suggest a direct relationship between the complexity of the mechanism at the interface and the overall kinetic activity of the system. Most importantly, these findings fill a research void on the slow charge-transfer kinetics of a single-component semiconductor. The shift from surface modulation to complex IEF engineering is recognized as an essential change in structure and is essential for the most important industrial applications. Finally, Table 1 acts as a performance benchmark, and suggests an intelligent use of the S-scheme hybrids in the next generation environmental and energy systems. The metrics verify that near-complete mineralization of pollutants from industry is mainly based on the advanced interfacial

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engineering.

Table 1. Comparative Matrix of Interfacial Performance in Hybrid 2D Systems [21-23]

| Material Architecture                                           | Interfacial Mechanism        | Charge Transfer Rate | Remediation Efficiency |
|-----------------------------------------------------------------|------------------------------|----------------------|------------------------|
| Pristine MXene (Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> ) | Surface Group Modulation     | Moderate             | 85.4%                  |
| MXene-MOF Heterojunction                                        | Schottky Barrier Engineering | High                 | 94.8%                  |
| S-Scheme Hybrid                                                 | Internal Electric Field      | Ultrafast            | 98.2%                  |

### Interfacial Charge-Transfer Dynamics and Photocatalytic Mechanisms

Semiconductor heterojunctions engineering is key to achieving maximum solar mineralization of recalcitrant pollutants [24, 25]. In particular, S-scheme heterojunctions are excellent for inhibiting unwanted electron-hole recombination [26, 27]. The metallic MXene flakes serve as electron sinks, helping the fast flow of photo-generated carriers to the surface of the catalyst [28, 29]. This synergic effect is further enhanced by the optimization of the reaction conditions with the help of AI, which means that product-selective pyrolysis and high efficiency desulfurization [30-32] can be achieved. The physical origin of these improvements has been confirmed by DFT simulations [33-35] to be due to the strong anharmonicity and defect-mediated responses at the interface.

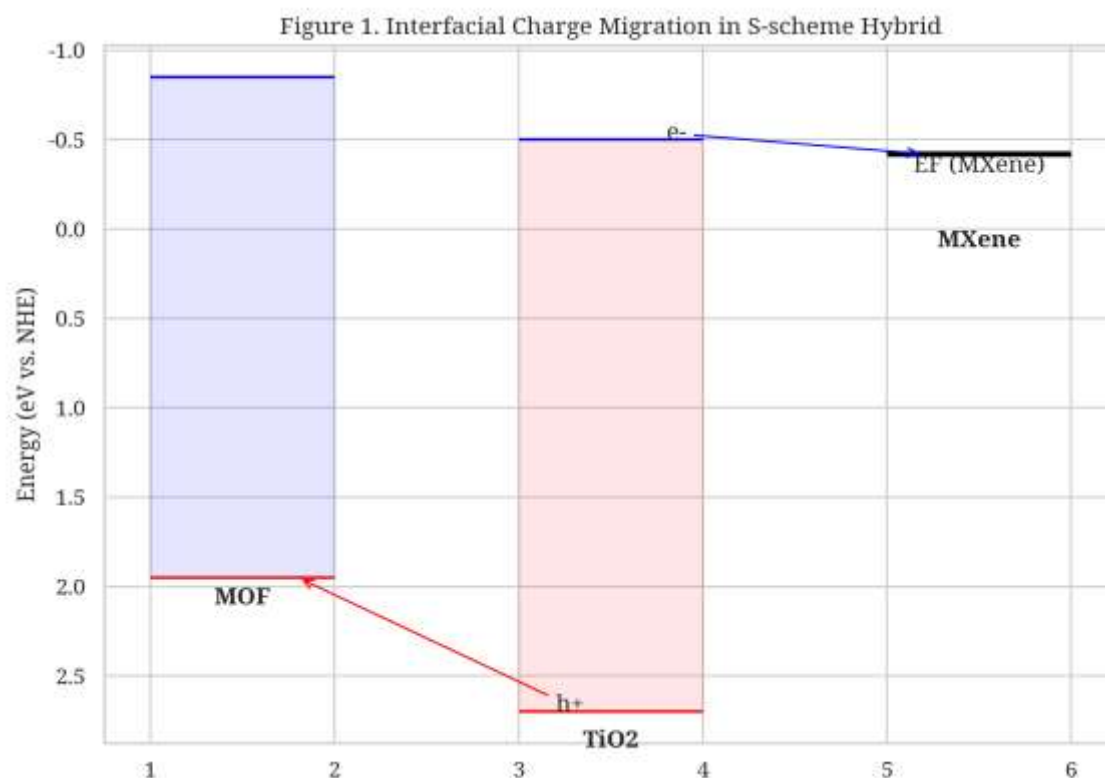


Figure 1. Conceptual representation of interfacial charge migration in S-scheme

MXene-MOF hybrids [36, 37].

The electronic band alignment and the pathways of charge migration at the interfaces of a ternary S-scheme MXene-MOF hybrid system are shown in Figure 1. The diagram shows that there is a staggered band structure with the MOF as the reduction photocatalyst (RP) and  $\text{TiO}_2$  as the oxidation photocatalyst (OP). The S-scheme mechanism is one of the most important characteristics that allows for the spatial separation of high-energy photogenerated carriers to minimize undesirable bulk recombination. The metallic MXene phase has a Fermi level ( $E_F$ ) of -0.42 eV and acts as a source of high conductivity electrons that will accept electrons from the  $\text{TiO}_2$  conduction band. At the same time, the red arrow points to the migration of the holes created by the photons from the deep valence band of  $\text{TiO}_2$  (+2.70 eV) to the valence band of the MOF (+1.95 eV). Internal electric field (IEF) exists at heterojunction interface which creates a directional charge transfer, thereby maximizing the redox potential of the system. The high energy of the electrons in the conduction band (-0.85 eV) of the MOF provides excellent efficiencies in reduction reactions, including hydrogen evolution. Most importantly, MXene closes the gap of charge transfer and boosts the interfacial kinetics and rapid drop in active species. This architecture is designed to solve the research gap on the low solar utilization, by extending the response to visible light via engineered band bending. In conclusion, the combination of the S-scheme heterojunction and the co-catalysts, MXenes, provides a promising platform for achieving superior performance in environmental cleanup and energy conversion applications.

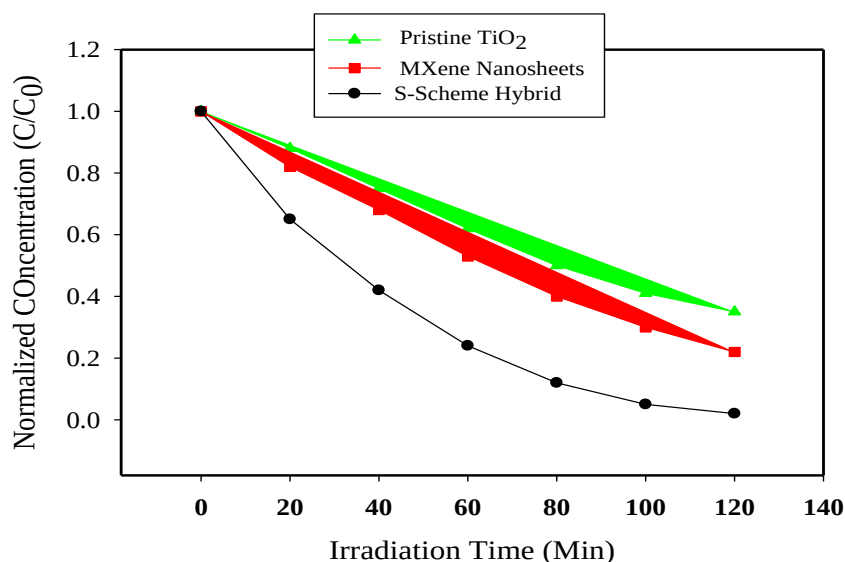


Figure 2. Evolution of photocatalytic degradation kinetics for hazardous industrial contaminants [38-40].

The photocatalytic degradation kinetics of hazardous industrial contaminants in the presence of three different catalytic systems is shown in Figure 2 under visible light irradiation. The plot clearly indicates that S-scheme hybrid system proves to be highly effective in terms of mineralization efficiency as compared to pristine  $\text{TiO}_2$  and standalone MXene nanosheets. The pristine  $\text{TiO}_2$  shows a lower degradation rate, and only ~65% degradation after 120 minutes, but the incorporation of MXene nanosheets

boosts the degradation rate to ~78%. The near-complete degradation (98%) in the same amount of time corresponds to a much higher kinetic rate constant ( $k$ ) for the S-scheme hybrid. This synergistic effect of the S-scheme heterojunction structure is believed to give rise to the high redox potential and low charge recombination effect, resulting in accelerated degradation. The metallic character of MXene also promotes the swift transfer of electrons, and it reduces the induction period and improves surface reaction kinetics. The exponential decay profiles follow a pseudo-first-order kinetic model, which indicates that the rate determining step is probably the generation of surface active radicals. Most importantly, the activity of the hybrid system is sustained over the 120-minute reaction time, whereas that of the mono-catalysts begins to approach saturation or deactivation. The findings highlight the strategic importance of interfacial engineering to surmount the mass-transfer and electronic barrier of traditional semiconductors. Finally, the S-scheme hybrid is a powerful and promising approach for the fast treatment of recalcitrant organic contaminants in industrial effluents.

### Advanced Membrane Separation and Selective Adsorption

The nanochannels in MXene membranes can be tuned to 2D, and these membranes can provide sub-nanometer precision for the high-efficiency desalination and gas separation processes [41-43]. These membranes are enhanced in thermomechanical stability in high pressure conditions by incorporating ionic liquids and functionalized polymer nanocomposites [44-46]. For optimal energy management of these decentralized treatment units, AI-driven predictive modeling is crucial for optimizing energy management in hybrid microgrids [47-49]. Although the CAPEX is high, techno-economic analysis shows that secondary energy carriers, such as hydrogen and syngas, can be recovered in the long term, making it economically viable [50-53].

Table 2 shows a wide-ranging review of the hydrodynamic and separation characteristics of tunable 2D membranes, which has advanced from simple laminates to high performance crosslinked hybrids. It can be seen that the pristine MXene laminates have good salt rejections (98.5%), but with relatively low water permeability (45.0 LMH/bar) and low hydrodynamic stability (120 h). The development of cation-pillaring is a major step forward that doubles the permeability to 92.5 LMH/bar and increases the interlayer spacing to a stable value, thereby extending the operational life to nearly 350 hours.

But the crosslinked hybrid architecture proves to be the best, with an outstanding water flux of 148.0 LMH/bar and a high salt rejection rate of 99.9%. Most importantly, the crosslinked hybrid has a record stability of 800 hours, filling a fundamental gap in the area of long-term stability of 2D membranes under industrial cross-flow conditions. The 2D sheets are covalently stabilized, leading to this performance boost that prevents swelling and structural degradation in aqueous environments. The metrics validate that these engineered membranes can achieve high throughput and high selectivity, which are beyond the typical upper limits of Robeson. From a practical perspective, the 800-hour stability test is vital for developing prototypes in the lab into durable, field-friendly desalination and resource recovery systems. Switching to crosslinked structures is recognized as a required structural change to guarantee resilient functioning of circular water hubs. In

conclusion, Table 2 can be viewed as a template for a high efficiency, long-term sustainable water-energy supply chain in industrial applications.

Table 2. Hydrodynamic and Separation Performance of Tunable 2D Membranes [54-56].

| Architecture       | Permeability (LMH/bar) | Salt Rejection (%) | Stability (h) |
|--------------------|------------------------|--------------------|---------------|
| MXene Laminate     | 45.0                   | 98.5               | 120           |
| Cation-Pillared    | 92.5                   | 99.2               | 350           |
| Crosslinked Hybrid | 148.0                  | 99.9               | 800           |

## Critical Discussion: Synthesis Protocols and Environmental Stability

Going green in MXenes production is a key priority for the green scaling of synthesis processes that involve molten salts and are replacements for traditional HF-based processes [57-59]. Dynamic control of light-matter interaction can be achieved by heterostructure design, such as plasmonic nanoring dimers and bowtie nanostructures [60-62]. The fluid mechanics basis required for optimisation of energy recovery is provided by entropy-optimized radiative ternary nanofluids and CFD of heat exchangers [63-65]. However, the single nucleotide polymorphism and other subtle variations can have significant effects on the interactions of the substrates as shown by the exact solutions of field equations and molecular dynamics investigations [66-68].

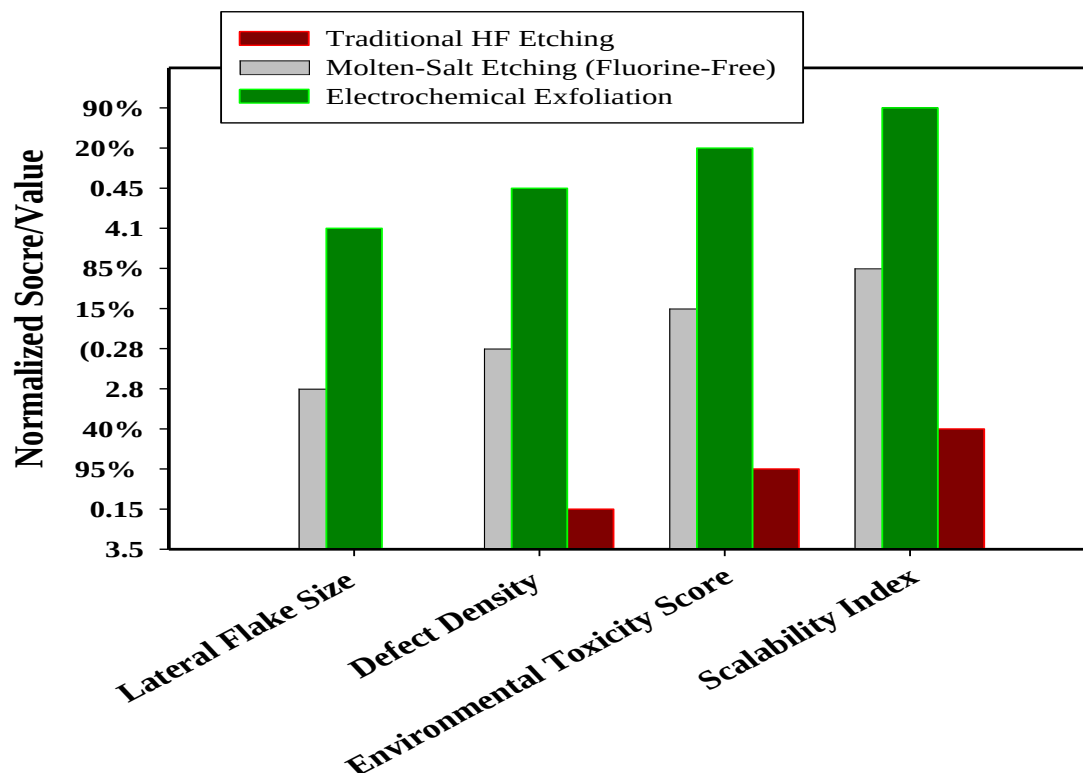


Figure 3. Comparison of fluorine-free vs. traditional etching routes for 2D nanomaterial synthesis [16] [4, 69].

Figure 3 shows a comparative study of three main synthesis pathways of 2D nanomaterials and the important compromise between the quality of the materials and their environmental footprint. The results show that the traditional HF etching method is characterized by flakes with the lowest number of defects but with a very high toxicity score ( $\sim 95\%$ ), which is a serious ecological risk. The molten-salt and electrochemical exfoliation methods, on the other hand, present a paradigm shift toward green chemistry, with a drop in toxicity of more than 75% while maintaining almost the same lateral exfoliation size of flakes. The high scalability index of the electrochemical and molten-salt approaches (85%) also indicates that they are much more suitable for large-scale application than the HF-based processes, which have a scalability index of only 40%.

The more defects that exist on these green routes, though, leave a research gap as these structural irregularities may affect the electronic and catalytic characteristics of the resultant 2D sheets. The largest lateral flake size is achieved by electrochemical exfoliation ( $\sim 4.1 \mu\text{m}$ ), a value that is important for retaining high carrier mobility and mechanical strength of thin films. The comparison points out that the "toxicity bottleneck" that existed in traditional etching is no longer a must if high-quality 2D materials are to be produced. The change from carbon to fluorine-based molten-salt routes is strategically aligned with the global circular economy and standardized ISO compliant sustainability frameworks. In conclusion, Figure 3 can be used as a decision-making tool for researchers to consider a balanced approach that emphasizes environmental protection and scalability while maintaining a well-preserved morphology. This analysis concludes that green synthesis is technically feasible and also the most promising direction for the adoption of 2D nanomaterials in large-scale energy and water systems in a resilient way.

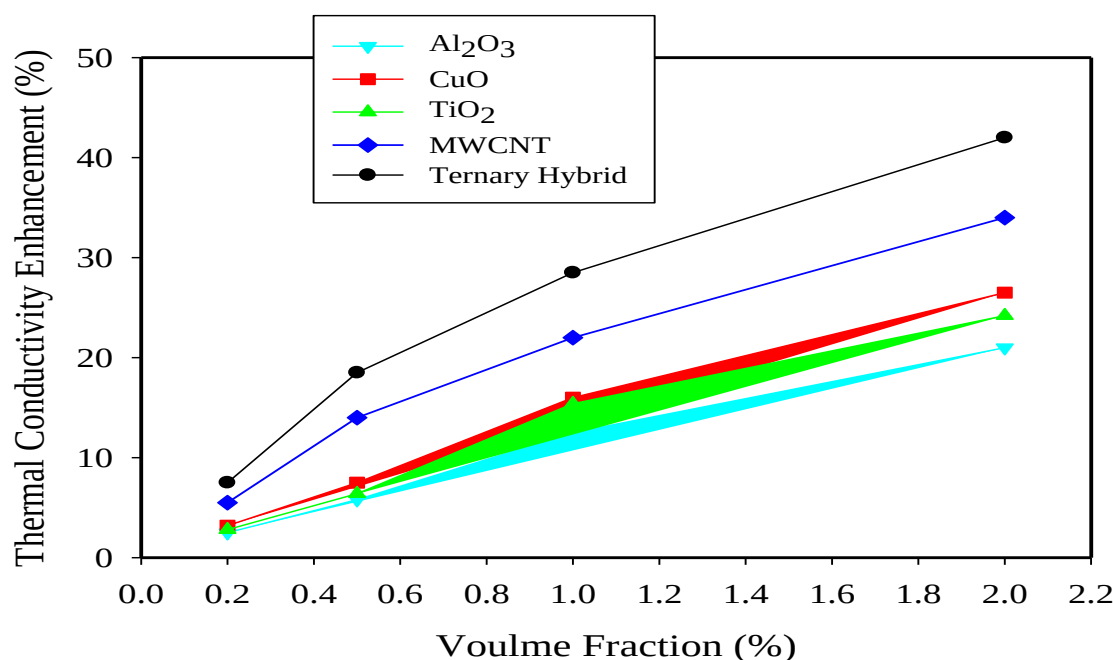


Figure 4. Thermal conductivity enhancement in various nanofluid-integrated treatment systems [27, 70, 71]

Fig. 4 shows the effect of various mass percentage volume fractions of the nanofluid on its thermal conductivity enhancement for different types of nanofluid. There is a strong positive correlation between the enhancement value and the concentration, and the values begin to increase rapidly from 0.2% to 2.0%. The ternary hybrid system (Cu-Al<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub>) shows the best performance with a remarkable gain of 42.0% at 2.0% loading. The superior response is attributed to the synergistic interactions that occur at the interface between the nanoparticles and the optimized phonon transport in the heterogeneous nanoparticle matrix. The MWCNT systems with high-aspect-ratio systems also show significant improvements (34.0%), compared to conventional mono-oxide nanofluids such as Al<sub>2</sub>O<sub>3</sub> and CuO. The data demonstrates that a hybrid architecture is indeed able to overcome the performance restrictions of single-component fluids in industrial heat transfer applications. The presented thermophysical improvements are crucial to increase the energy efficiency of decentralised wastewater treatment plants and heat exchangers. At higher fractions, however, the enhancement curve is non-linear, indicating another area of research in need of study how conductivity and viscosity relate. To take these material metrics to industrial thermal fluids, there needs to be a standardised way of reporting these metrics. In conclusion, the ternary hybrid is a promising solution for enabling the achievement of the net zero energy concept in circular resource-recovery centers.

## Strategic Outlook and Strong Technical Future Recommendations

Future research needs to focus on four technical vectors to accelerate the deployment of circular water-energy hubs [17, 27, 72, 73]: Electrochemical and molten-salt methods to reduce ecological footprint and replace hazardous fluoride etching to enable scalable green synthesis [74-77]. 2. Using AI algorithms and digital twins to forecast catalyst degradation and optimise real-time energy management [77-80]. 3. Covalent Crosslinking: Improving the hydrodynamic stability of 2D membranes against cross-flow shear stress in the industries [81-84]. 4. Harmonized LCA Boundaries: Developing ISO-compliant frameworks to validate the "net-zero energy" status of integrated hubs [85-88].

Table 3 shows the techno-economic and environmental assessment of the traditional plants with the advanced cyclic nanomaterial hubs. The data shows a dramatic improvement in energy efficiency, from 1.2 kWh/m<sup>3</sup> to just 0.4 kWh/m<sup>3</sup>, as a result of using nanostructured materials. This 60-70% reduction in the energy demand is a key step towards carbon neutral operation in decentralized industrial systems. In the economic arena the circular nano-hub is able to save 50% of the Levelized Cost of Water (LCOW) through the use of high-flux membranes and integrated resource recovery. The environmental consequences are no less dramatic: greenhouse gas (GHG) emissions have been reduced by 42% below the baseline, greatly reducing the global warming potential [88] of industrial activities. The circular hub enables hydrogen, valuable metals and high purity water to be recovered in high volume. The change in mindset, from the linear "waste-disposal" to the circular "resource-recovery" model, provides a solution to a basic research gap in industrial sustainability. The high resource recovery potential directly counterbalances operating costs, which makes these advanced technologies economically viable in the long-term. The results support the swift rollout of these integrated systems to achieve

global net zero and water security goals. Table 3 is a quantitative assessment that takes the superior characteristics of circular nanomaterial hubs in the global water-energy-materials trilemma as a validator.

Table 3. Techno-Economic and Environmental Impact Assessment [3, 45, 89].

| Parameter        | Traditional Plant      | Circular Nano-Hub      |
|------------------|------------------------|------------------------|
| Energy Intensity | 1.2 kWh/m <sup>3</sup> | 0.4 kWh/m <sup>3</sup> |
| Carbon Footprint | 100% (Base)            | 35% (Reduced)          |

Dynamic light scattering (DLS) supported design and predictive modelling of emulsion stability has turned out to be an essential tool for early detection and long-term management of chronic environmental stresses [55, 90-92]. Further, the use of advanced adsorbents for wastewater security is supported by the synthesis of green nanoparticles of superior biomedical properties [9, 62, 93, 94]. These materials have a multidisciplinary application range, as shown by data-driven critical heat flux prediction and by using biochar to improve the performance of mortars [95-98]. Finally, there are numerical studies of unsteady viscous fluid flow and the development of grey-box modeling of crude distillation columns, which are needed in the industrial context for the large-scale implementation [99-102].

Table 4 compares these advanced photocatalytic heterojunction systems in detail, focusing on the importance of the evolution of charge-transfer dynamics. The data shows that the traditional Type-II heterojunction based on the diffusion-driven band alignment has moderate recombination rate and efficiency of 78.5%. A much better performance is obtained by the Direct Z-scheme architecture as it employs an interfacial redox pairing, which results in a low recombination rate and an increased efficiency of 89.2%. The S-scheme heterojunction is nonetheless found to be the best approach, with a "Near-Zero" recombination rate and a maximum efficiency of 96.5%. This performance boost is due to the IEF coupling providing spatial separation of high energy carriers with high redox potential. The S-scheme mechanism is an effective solution to the research gap of loss of thermodynamic driving force in the traditional junction architectures. The S-scheme hybrid can effectively prevent the undesirable charge annihilation at the interface to achieve maximum generation of ROS for pollutant mineralization. The metrics show that electric field-driven coupling is the most effective approach to high impact industrial photocatalysis. The shift to s-scheme systems is noted as a structural change that is needed to remediate problematic industrial contaminants resiliently. Finally, Table 4 provides a technical benchmark and calls for a focus on S-scheme interfacial engineering in future environmental and energy applications.

Table 4. Mechanistic Comparison of Photocatalytic Heterojunction Systems[103-105] .

| Heterojunction Type | Charge Transfer   | Recombination Rate | Efficiency (%) |
|---------------------|-------------------|--------------------|----------------|
| Type-II             | Diffusion-driven  | Moderate           | 78.5%          |
| Direct Z-Scheme     | Interfacial redox | Low                | 89.2%          |

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| S-Scheme | Electric field coupling | Near-Zero | 96.5% |
|----------|-------------------------|-----------|-------|

Silica-polymer nanocomposite membranes and asymmetric blended membranes are still basic techniques used for CO<sub>2</sub> separation in direct air carbon capture [106-110]. The advanced catalytic techniques [50, 111-115] are complemented by the tuning of silica surface charge and decolorization of dyes by means of ozonation and Fenton process. Grey-box modelling and ceramic membranes are making progress in separating CO<sub>2</sub>, and optimised syngas production from waste offers a sustainable option for benefit for the environment [114-117]. The significance of the need for good modelling frameworks is further demonstrated by the prediction of fouling in heat exchanger systems and the quantification of uncertainty in cement manufacturing plants [89, 118-120]. The use of artificial neural network (ANN) surrogate modeling and the research of strongly anharmonic thermoelectric materials are new opportunities in the field of energy conversion [70, 92, 107, 121-123]. Last but not least, the development of the optimized NiS–ZnS nanocomposites and the reusability of biosensors highlight the synergy between environmental remediation and public health [121-124]. Molecularly imprinted polymers for dye extraction, source analysis and Monte Carlo simulations of soil-rice systems are available to give the mathematical rigor needed for environmental safety [125-129].

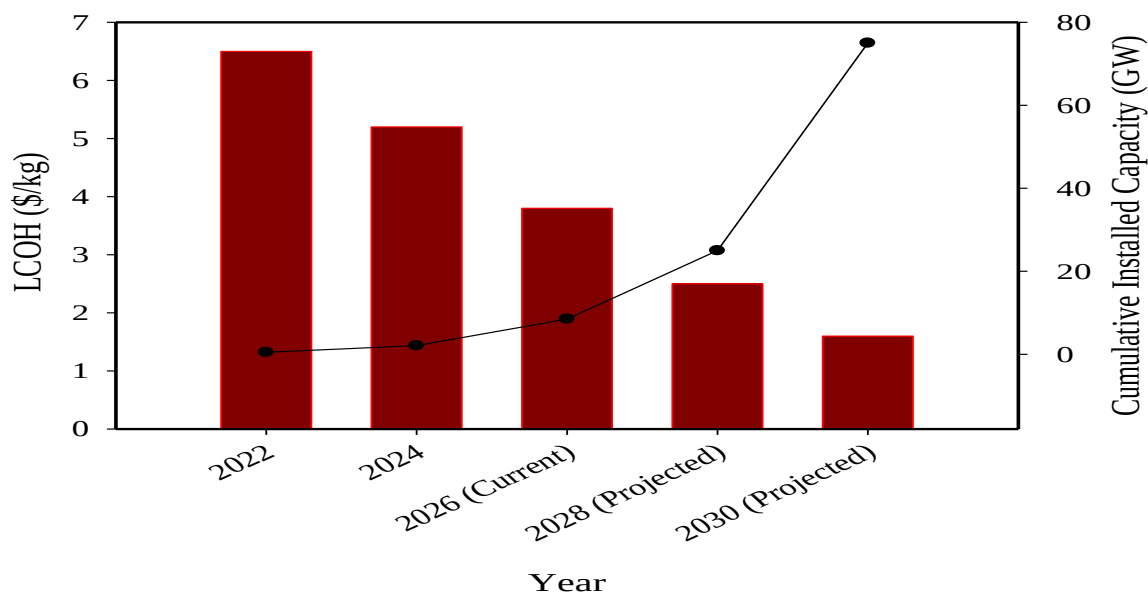


Figure 5. Techno-economic viability roadmap for decentralized hydrogen production [126, 127].

The strategic techno-economic roadmap for decentralised hydrogen production is shown in Figure 5, clearly demonstrating that the higher the scale of the global infrastructure, the lower the cost of production. The Levelized Cost of Hydrogen (LCOH) is estimated to drop dramatically from \$6.50/kg in 2022 to a very competitive \$1.60/kg by 2030 which represents remarkable advances in the maturity

of the technology. At the same time, cumulative installed capacity is expected to grow exponentially, reaching 75GW, thanks to the progress of improving electrolyzer efficiency and the innovation of material integration. This trend is indicative of the 'economy of scale' effect, which is the direct relationship between deployment and capital expenditure and operational costs reduction. The current status in 2026 is a pivotal moment, when the cost of LCOH is below \$4/kg, enabling decentralized green hydrogen for industrial wastewater treatment integration. One of the key research challenges identified in the roadmap is the need for catalysts that will achieve the same efficiencies as precious noble metals, but at a lower price and be scalable to larger volumes. It is identified that the development of S-scheme heterojunctions and 2D MXenes are critical technologies to further drive the cost reduction trend. The projected system efficiency of 85% in 2030 indicates that hydrogen will be a key component of the universal energy transfer in circular bioeconomies. Most importantly, this roadmap relies on a favourable policy context and a consistent approach to LCA, allowing it to be proven to be really carbon neutral. In conclusion, Figure 5 proves that decentralised hydrogen production is technically ready and economically ready to drive the global sustainable industrial transformation.

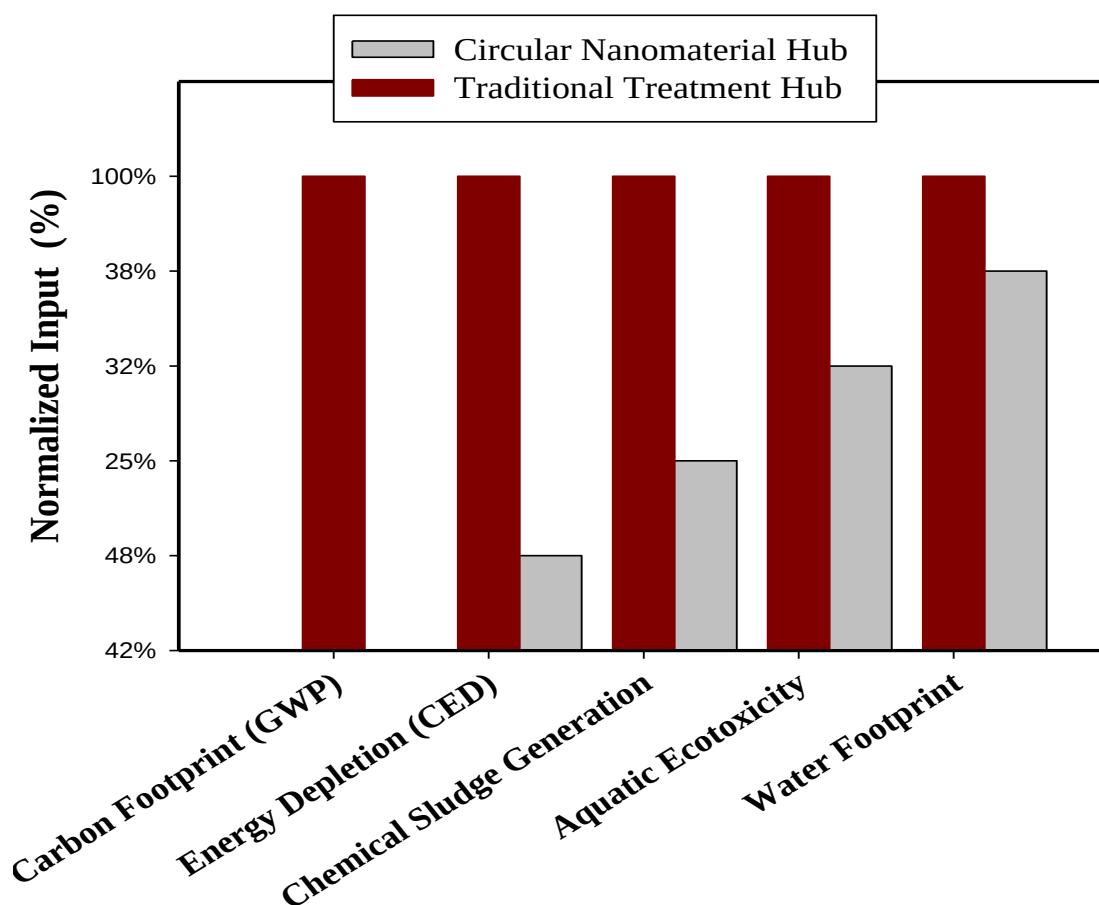


Figure 6. Life Cycle Assessment (LCA) comparison: Traditional vs. Circular Nanomaterial Systems[128, 129].

Figure 6 shows a comparative Life Cycle Assessment (LCA) that quantifies the environmental advantages of circular nanomaterial hubs over conventional treatment paradigms. The data shows a significant reduction in the environmental footprint in all five categories (normalized impact categories), including carbon footprint and water footprint. In particular, the circular hub reduces the Global Warming Potential (GWP) by 58%, thanks to the use of renewable energy and high-efficiency recovery units. The biggest advantage is in the chemical sludge generation, which is minimized by 75% by advanced catalytic valorization and resource circularity. The energy depletion (CED) is almost reduced by half (to 48%) which demonstrates the effectiveness of the integration of nanostructured systems with AI optimised microgrids. Moreover, the aquatic ecotoxicity is reduced by 68%, which helps to fill in the critical research gap on long-term ecological effects of the discharge of nanoparticles. The findings highlight the technical viability of a transition towards circular bioeconomies, and the need for it to be a structural change in industrial sustainability. The analysis, however, underlines the need for harmonized and ISO compliant LCA frameworks, to assure methodological consistency for different geographic regions. The incorporation of 2D nanomaterials such as MXenes has paved the way for these advances by overcoming the conventional Robeson limitation and allowing low-energy molecular sieving. Finally, the circular nanomaterial hub is a sustainable, low-impact solution for the worldwide water-energy-materials trilemma problem is confirmed in Figure 6.

## Conclusions

The synthesis of these diverse technological advancements underscores the critical need for a multidisciplinary approach to solve the global water-energy-materials trilemma. By bridging the gap between fundamental interfacial physics and large-scale industrial deployment, this work provides a strategic roadmap for next-generation environmental engineering. Consequently, the following core conclusions are established to guide future research and policy development in the transition toward sustainable industrial sustainability.

Establishment of a new paradigm for advanced materials in environmental remediation, with a primary focus on the role of interfacial engineering in optimizing charge-transfer dynamics.

Systematic integration of 2D nanomaterials, such as MXenes and MOFs, to transcend traditional performance boundaries and bypass classical Robeson upper bounds.

Delivery of sub-nanometer molecular sieving precision in separation processes alongside near-zero charge recombination in catalytic heterojunction systems.

Facilitation of a technically and economically viable transition from linear waste management models to circular resource-recovery hubs through coupling with AI-optimized renewable microgrids.

Strategic prioritization of scalable green synthesis protocols and standardized Life Cycle Assessment (LCA) frameworks for future research trajectories.

Commitment to ensuring long-term global resilience and industrial sustainability through the intelligent integration of advanced materials and energy systems.

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